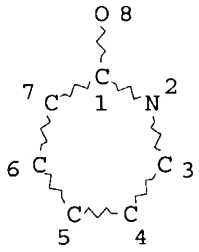
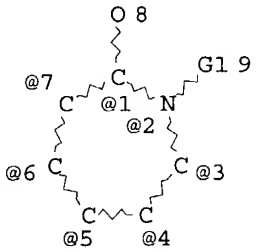
```
=> d que l103
L96             STR
```

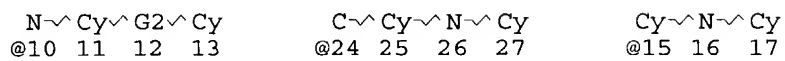


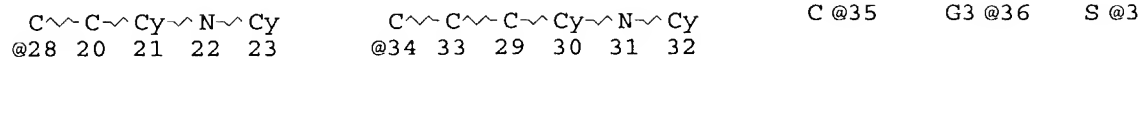

```
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L97       17246 SEA FILE=REGISTRY SSS FUL L96
L101            STR
```







Page 1-A

7

```
Page 1-B
VAR G1=15/10/24/28/34
REP G2=(0-4) 35
VAR G3=37/38
VPA 36-1/2/3/4/5/6/7 U
NODE ATTRIBUTES:
NSPEC   IS RC     AT  10
NSPEC   IS RC     AT  16
NSPEC   IS RC     AT  20
NSPEC   IS RC     AT  22
```

```
NSPEC   IS RC     AT  24
NSPEC   IS RC     AT  26
NSPEC   IS RC     AT  28
NSPEC   IS RC     AT  29
NSPEC   IS RC     AT  31
NSPEC   IS RC     AT  33
NSPEC   IS RC     AT  34
NSPEC   IS RC     AT  35
NSPEC   IS RC     AT  37
NSPEC   IS RC     AT  38
CONNECT IS E1  RC AT   8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   2
NUMBER OF NODES IS  35

STEREO ATTRIBUTES: NONE
L103          0 SEA FILE=REGISTRY SUB=L97 SSS FUL L101
```

```
=> fil lreg

FILE 'LREGISTRY' ENTERED AT 09:25:00 ON 03 DEC 2004
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LREGISTRY IS A STATIC LEARNING FILE

=> fil reg

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STRUCTURE FILE UPDATES:     1 DEC 2004  HIGHEST RN 791553-15-6
DICTIONARY FILE UPDATES:    1 DEC 2004  HIGHEST RN 791553-15-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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=> file stnguide

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> d que l74
L58                 STR
```
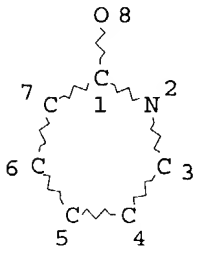



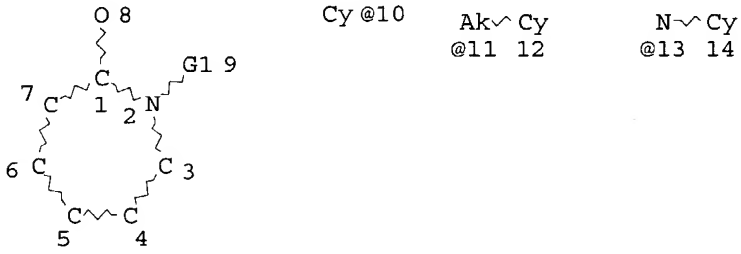
Case I

```
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   8
DEFAULT MLEVEL IS ATOM
```

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

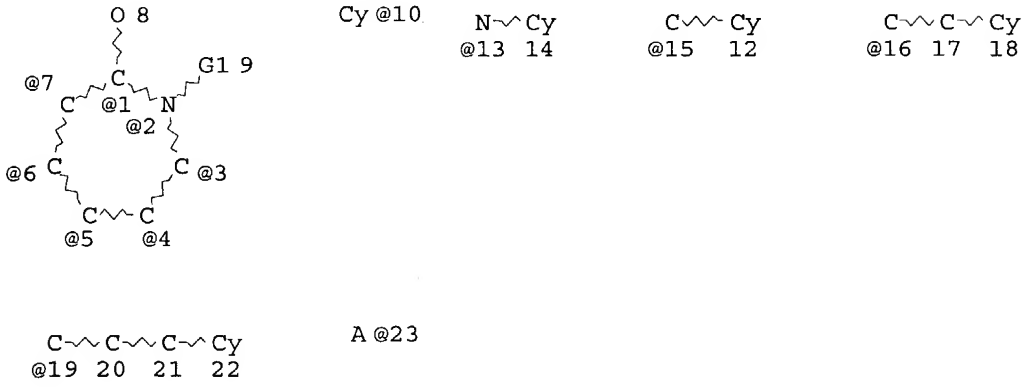
STEREO ATTRIBUTES: NONE
L59 (17246) SEA FILE=REGISTRY SSS FUL L58
L60 STR



VAR G1=10/11/13
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 10
GGCAT IS PCY AT 12
GGCAT IS PCY AT 14
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X9 C AT 11

GRAPH ATTRIBUTES:
RSPEC 2
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L61 141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L72 STR



VAR G1=10/13/15/16/19
VPA 23-1/2/3/4/5/6/7 U
NODE ATTRIBUTES:
NSPEC IS RC AT 13
NSPEC IS RC AT 15
NSPEC IS RC AT 16
NSPEC IS RC AT 17

```
NSPEC   IS RC     AT  19
NSPEC   IS RC     AT  20
NSPEC   IS RC     AT  21
NSPEC   IS RC     AT  23
CONNECT IS E1  RC AT   8
DEFAULT MLEVEL IS ATOM
GGCAT   IS PCY  AT  10
GGCAT   IS PCY  AT  12
GGCAT   IS PCY  AT  14
GGCAT   IS PCY  AT  18
GGCAT   IS PCY  AT  22
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   2
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
L74           29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72


=> fil reg

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STRUCTURE FILE UPDATES:     1 DEC 2004  HIGHEST RN 791553-15-6
DICTIONARY FILE UPDATES:    1 DEC 2004  HIGHEST RN 791553-15-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> analyze l74
ENTER ANSWER NUMBER OR RANGE (1-):1-
ENTER DISPLAY CODE (CHEM) OR ?:lc
L75           ANALYZE L74 1- LC :        9 TERMS

=> d
L75           ANALYZE L74 1- LC :        9 TERMS

TERM #    # OCC   # DOC   % DOC LC
------ -------- ------ ------ ---------------
     1       27     27  93.10 CA
     2       27     27  93.10 CAPLUS
     3       14     14  48.28 USPATFULL
     4       10     10  34.48 TOXCENTER
```

```
     5        4       4  13.79 CASREACT
     6        2       2   6.90 CHEMCATS
     7        1       1   3.45 IFICDB
     8        1       1   3.45 IFIPAT
     9        1       1   3.45 IFIUDB
*********  END OF L75***


=> file stnguide

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> => d que l85
L62              STR
```
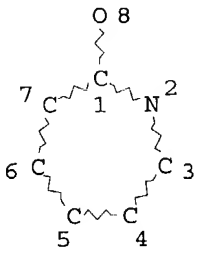
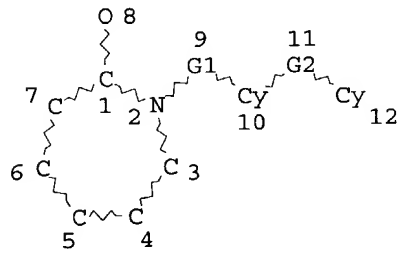



Case II

```
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L63 (     17246) SEA FILE=REGISTRY SSS FUL L62
L64              STR
```

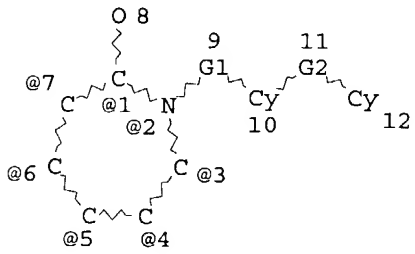



```
REP G1=(0-6) 13
REP G2=(0-6) 14
NODE ATTRIBUTES:
NSPEC   IS RC     AT  13
NSPEC   IS RC     AT  14
CONNECT IS E1  RC AT   8
```

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 2
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L65 647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L79 STR



C @13 C @14 G3 @15 S @16 CH2 @17

REP G1=(0-4) 13
REP G2=(0-4) 14
VAR G3=16/17
VPA 15-1/2/3/4/5/6/7 U
NODE ATTRIBUTES:
NSPEC IS RC AT 13
NSPEC IS RC AT 14
NSPEC IS RC AT 16
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 2
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L85 86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79

=>

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:53:16 ON 03 DEC 2004
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STRUCTURE FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6
DICTIONARY FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

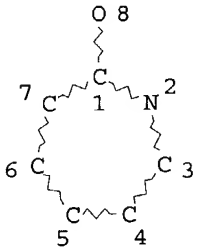
=> analyze l85
ENTER ANSWER NUMBER OR RANGE (1-):1-
ENTER DISPLAY CODE (CHEM) OR ?:lc
L86 ANALYZE L85 1- LC : 3 TERMS

=> d
L86 ANALYZE L85 1- LC : 3 TERMS

TERM #	# OCC	# DOC	% DOC	LC
1	86	86	100.00	CA
2	86	86	100.00	CAPLUS
3	30	30	34.88	USPATFULL

********* END OF L86***

=> d que l69
L66 STR

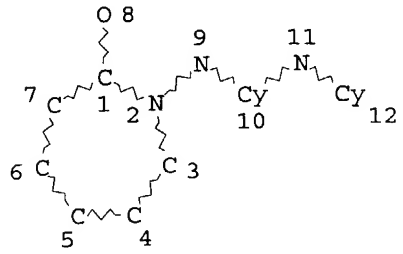


case III

NODE ATTRIBUTES:
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L67 (17246) SEA FILE=REGISTRY SSS FUL L66
L68 STR



NODE ATTRIBUTES:
NSPEC IS RC AT 9
NSPEC IS RC AT 11
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 2
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L69 0 SEA FILE=REGISTRY SUB=L67 SSS FUL L68

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 09:53:52 ON 03 DEC 2004
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> => fil hcap

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FILE COVERS 1907 - 3 Dec 2004 VOL 141 ISS 23
FILE LAST UPDATED: 1 Dec 2004 (20041201/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil uspatfull

FILE 'USPATFULL' ENTERED AT 10:00:10 ON 03 DEC 2004
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 2 Dec 2004 (20041202/PD)
FILE LAST UPDATED: 2 Dec 2004 (20041202/ED)
HIGHEST GRANTED PATENT NUMBER: US6826778
HIGHEST APPLICATION PUBLICATION NUMBER: US2004244085
CA INDEXING IS CURRENT THROUGH 2 Dec 2004 (20041202/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 2 Dec 2004 (20041202/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2004

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

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=> fil casreact

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FILE CONTENT:1840 - 28 Nov 2004 VOL 141 ISS 22

****
*
* CASREACT now has more than 8 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil toxcenter

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FILE COVERS 1907 TO 30 Nov 2004 (20041130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

TOXCENTER has been enhanced with new files segments and search fields. See HELP CONTENT for more information.

TOXCENTER thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2004 vocabulary. See http://www.nlm.nih.gov/mesh/ and http://www.nlm.nih.gov/pubs/techbull/nd03/nd03_mesh.html for a description of changes.

```
=> file stnguide
FULL ESTIMATED COST                                    0.61      374.71

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> d que nos l89
L58              STR
L59 (     17246)SEA FILE=REGISTRY SSS FUL L58
L60              STR
L61         141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62              STR
L63 (     17246)SEA FILE=REGISTRY SSS FUL L62
L64              STR
L65         647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72              STR
L74          29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79              STR
L85          86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L87          19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L74
L88           4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L85
L89          22 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L87 OR L88


=> d que nos l92
L58              STR
L59 (     17246)SEA FILE=REGISTRY SSS FUL L58
L60              STR
L61         141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62              STR
L63 (     17246)SEA FILE=REGISTRY SSS FUL L62
L64              STR
L65         647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72              STR
L74          29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79              STR
L85          86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L90           6 SEA FILE=USPATFULL ABB=ON  PLU=ON  L74
L91           1 SEA FILE=USPATFULL ABB=ON  PLU=ON  L85
L92           7 SEA FILE=USPATFULL ABB=ON  PLU=ON  (L90 OR L91)


=> d que nos l93
```

```
L58              STR
L59 (      17246)SEA FILE=REGISTRY SSS FUL L58
L60              STR
L61          141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62              STR
L63 (      17246)SEA FILE=REGISTRY SSS FUL L62
L64              STR
L65          647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72              STR
L74           29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79              STR
L85           86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L93            2 SEA FILE=CASREACT ABB=ON  PLU=ON  L74 OR L85


=> d que nos l94
L58              STR
L59 (      17246)SEA FILE=REGISTRY SSS FUL L58
L60              STR
L61          141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62              STR
L63 (      17246)SEA FILE=REGISTRY SSS FUL L62
L64              STR
L65          647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72              STR
L74           29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79              STR
L85           86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L94           10 SEA FILE=TOXCENTER ABB=ON  PLU=ON  L74 OR L85


=> dup rem l89 l92 l93 l94

FILE 'HCAPLUS' ENTERED AT 10:01:06 ON 03 DEC 2004
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FILE 'TOXCENTER' ENTERED AT 10:01:06 ON 03 DEC 2004
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PROCESSING COMPLETED FOR L89
PROCESSING COMPLETED FOR L92
PROCESSING COMPLETED FOR L93
PROCESSING COMPLETED FOR L94
L95           30 DUP REM L89 L92 L93 L94 (11 DUPLICATES REMOVED)
                 ANSWERS '1-21' FROM FILE HCAPLUS
                 ANSWERS '22-26' FROM FILE USPATFULL
                 ANSWERS '27-30' FROM FILE TOXCENTER

=> d ibib abs ed hitstr 1-21

L95  ANSWER 1 OF 30  HCAPLUS  COPYRIGHT 2004 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2003:837735  HCAPLUS
```

DOCUMENT NUMBER: 140:59238
TITLE: Unusual Tethering Effects in the Schmidt Reaction of Hydroxyalkyl Azides with Ketones: Cation-π and Steric Stabilization of a Pseudoaxial Phenyl Group
AUTHOR(S): Katz, Christopher E.; Aube, Jeffrey
CORPORATE SOURCE: Department of Chemistry, University of Kansas, Lawrence, KS, 66045-7582, USA
SOURCE: Journal of the American Chemical Society (2003), 125(46), 13948-13949
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:59238

AB The Lewis acid-promoted reactions of chiral 2-aryl-3-azido-1-propanols with 4-substituted cyclohexanones lead to iminium ethers and ultimately caprolactams (following a hydrolysis step). In this study, it is shown that these reactions afford variable ratios of products, depending on the electronic nature of the Ph group. These results are interpreted in the context of a cation-π stabilizing effect in the product-determining reaction intermediate. Remarkably, the best selectivity was obtained when an azidopropanol reagent containing a quaternary center was used; a control experiment showed that the high selectivity observed in this result depended upon the free rotation of the pseudoaxial aromatic group in the intermediate that affords the major product.

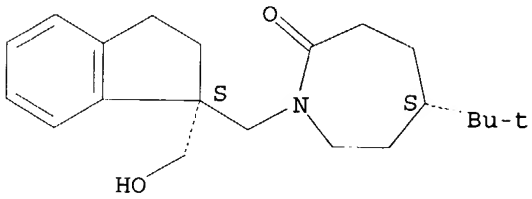
ED Entered STN: 27 Oct 2003

IT **637357-23-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(unusual tethering effects in Schmidt reaction of hydroxyalkyl azides with ketones)

RN 637357-23-4 HCAPLUS

CN 2H-Azepin-2-one, 1-[[(1R)-2,3-dihydro-1-(hydroxymethyl)-1H-inden-1-yl]methyl]-5-(1,1-dimethylethyl)hexahydro-, (5R)-rel- (9CI) (CA INDEX NAME)

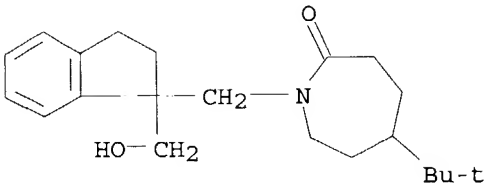
Relative stereochemistry.



IT **637356-71-9P 637356-73-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(unusual tethering effects in Schmidt reaction of hydroxyalkyl azides with ketones)

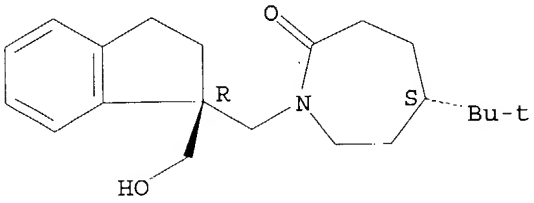
RN 637356-71-9 HCAPLUS

CN 2H-Azepin-2-one, 1-[[2,3-dihydro-1-(hydroxymethyl)-1H-inden-1-yl]methyl]-5-(1,1-dimethylethyl)hexahydro- (9CI) (CA INDEX NAME)



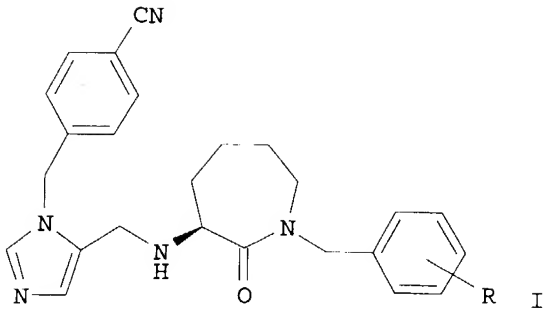
RN 637356-73-1 HCAPLUS
CN 2H-Azepin-2-one, 1-[[(1R)-2,3-dihydro-1-(hydroxymethyl)-1H-inden-1-yl]methyl]-5-(1,1-dimethylethyl)hexahydro-, (5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2003:462563 HCAPLUS
DOCUMENT NUMBER: 140:42082
TITLE: Parallel liquid synthesis of N,N'-disubstituted 3-aminoazepin-2-ones as potent and specific farnesyl transferase inhibitors
AUTHOR(S): Le Diguarher, Thierry; Ortuno, Jean-Claude; Dorey, Gilbert; Shanks, David; Guilbaud, Nicolas; Pierre, Alain; Fauchere, Jean-Luc; Hickman, John A.; Tucker, Gordon C.; Casara, Patrick J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Institut de Recherches Servier, Croissy sur Seine, 78290, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(14), 3193-3204
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:42082
GI



I

AB A rapid structure-activity study was performed by parallel liquid synthesis on N,N'-disubstitution of 3-aminoazepin-2-one to afford potent and specific farnesyl transferase inhibitors with low nM enzymic and cellular activities. The activities of the selected compds. were validated in vivo, and compds. I (R = 2-Cl, 3-Br) presented significant antitumor activity.

ED Entered STN: 17 Jun 2003

IT **635753-79-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(N,N'-disubstituted 3-aminoazepin-2-ones as farnesyl transferase inhibitors)

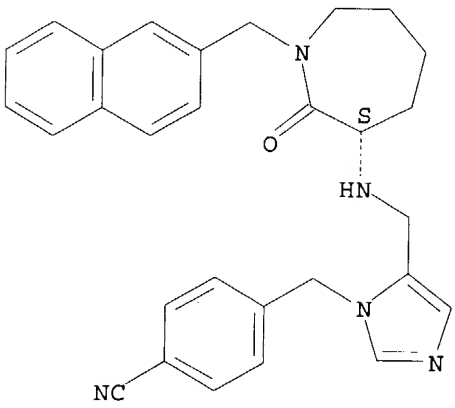
RN 635753-79-6 HCAPLUS

CN Benzonitrile, 4-[[5-[[[(3S)-hexahydro-1-(2-naphthalenylmethyl)-2-oxo-1H-azepin-3-yl]amino]methyl]-1H-imidazol-1-yl]methyl]-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 443920-60-3
CMF C29 H29 N5 O

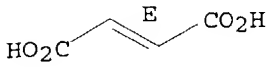
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

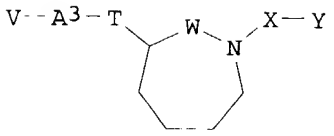


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

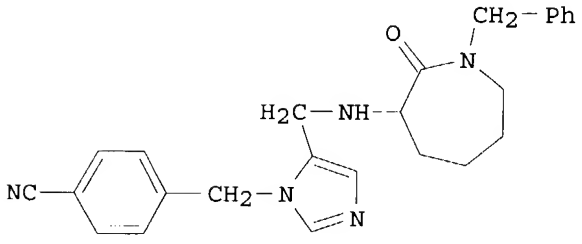
L95 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2002:555454 HCAPLUS
DOCUMENT NUMBER: 137:125097
TITLE: Novel azepanes as farnesyl transferase inhibitors
INVENTOR(S): Casara, Patrick; Le Diguarher, Thierry; Dorey, Gilbert; Hickman, John; Pierre, Alain; Tucker, Gordon; Guilbaud, Nicolas; Ortuno, Jean-Claude; Fauchere, Jean-Luc
PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057223	A2	20020725	WO 2002-FR147	20020116
WO 2002057223	A3	20021128		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
FR 2819511	A1	20020719	FR 2001-638	20010118
PRIORITY APPLN. INFO.:			FR 2001-638 A	20010118

OTHER SOURCE(S): MARPAT 137:125097
GI



I



II

AB Title compds. I [W = CO, CH2; X = bond, alkylene, CO, S(O)n, S(O)nA1, COA1, A1S(O)nA2, A1COA2; Y = (un)substituted aryl, heteroaryl, cycloalkyl, heterocyclalkyl; T = NR1, NR1CO; V = H, (un)substituted aryl, heteroaryl; A1, A2 = alkylene; A3 = (CR2R3)p; R1-R3 = H, (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl; n = 0-2; p = 0-4] were prepared for use as farnesyl transferase inhibitors in the treatment of cancers, neurofibromatosis type 1, and restenosis after angioplasty or vascular surgery. Thus, (S)-3-amino-1-benzyl-2-azepanone was prepared from L-lysine in 4 steps and treated with 1-(4-cyanobenzyl)-1H-imidazole-5-carboxaldehyde, obtained by treating HOCH2COCH2OH with PhCH2NH2 and KSCN and oxidation of the resulting alc., to give the title compound II.

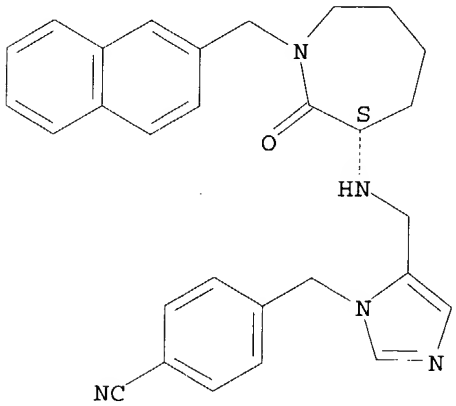
ED Entered STN: 26 Jul 2002

IT **443920-60-3P 443920-61-4P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(novel azepanes as farnesyl transferase inhibitors)

RN 443920-60-3 HCAPLUS

CN Benzonitrile, 4-[[5-[[[(3S)-hexahydro-1-(2-naphthalenylmethyl)-2-oxo-1H-azepin-3-yl]amino]methyl]-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443920-61-4 HCAPLUS

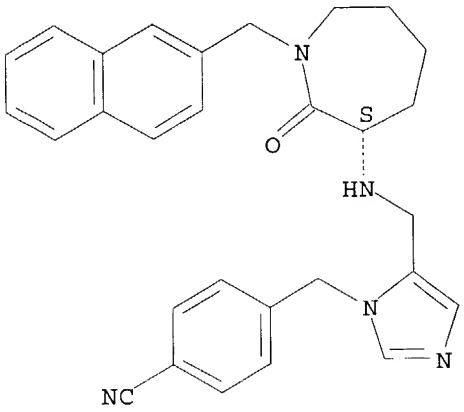
CN Benzonitrile, 4-[[5-[[[(3S)-hexahydro-1-(2-naphthalenylmethyl)-2-oxo-1H-

azepin-3-yl]amino]methyl]-1H-imidazol-1-yl]methyl]-, (2E)-2-butenedioate (5:7) (9CI) (CA INDEX NAME)

CM 1

CRN 443920-60-3
CMF C29 H29 N5 O

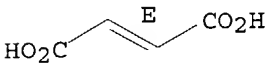
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



L95 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2002:571997 HCAPLUS
DOCUMENT NUMBER: 137:169533
TITLE: Preparation of microbiocidal N-phenyl-N-[4-(4-pyridyl)-pyrimidin-2-yl]amines
INVENTOR(S): Eberle, Martin; Ziegler, Hugo; Cederbaum, Fredrik; Ackermann, Peter
PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002053560	A1	20020711	WO 2001-XA2821	20011220

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,

LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PH, PL, PT, RO,
RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

WO 2002053560 A1 20020711 WO 2001-IB2821 20011220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GH, GM,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: GB 2001-102 A 20010103
WO 2001-IB2821 W 20011220

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

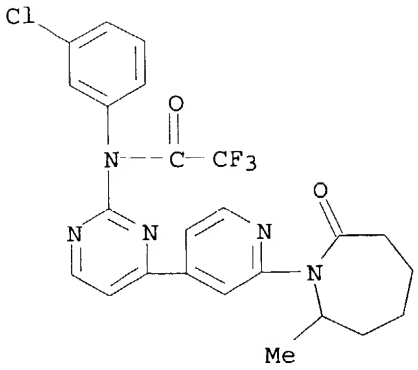
AB The title compds. [I; m + p = 0-3; n, q = 0-1, and m + p + q = 1-4; R1 = H, halo, alkoxy, haloalkyl, haloalkoxy, alkyl; R2 = H, alkyl, haloalkyl, alkoxy; R2a = H, alkyl, alkenyl, alkynyl; R3-R6 = H, alkyl, haloalkyl, hydroxyalkyl, alkoxyalkyl, or the ring members CR3R4 or CR5R6 or CR2R2a = CO, CS; X = CO, CS, SO, SO2; Y = O, S, CO, CH2, etc.; R7 = H, alkyl, alkenyl, etc.], useful in controlling or preventing the infestation of plants by phytopathogenic microorganisms, especially fungi, were prepared Thus,
treating 2-{4-[2-(3-chlorophenylamino)pyrimidin-4-yl]pyridin-2-ylamino}ethanol with phosgene afforded II which showed over 70% control against Pyrenophora teres on barley. This is part II of I-II series.

ED Entered STN: 02 Aug 2002

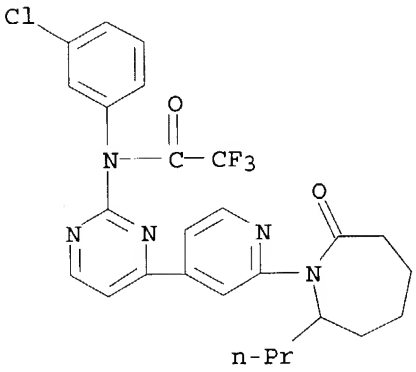
IT **448267-86-5P 448267-89-8P 448267-90-1P**
448270-89-1P 448270-92-6P 448270-93-7P
448274-18-8P 448274-21-3P 448274-22-4P
448277-11-0P 448277-14-3P 448277-15-4P
448280-06-6P 448280-09-9P 448280-10-2P
448283-17-8P 448283-20-3P 448283-21-4P
448286-23-5P 448286-26-8P 448286-27-9P
448289-56-3P 448289-59-6P 448289-60-9P
448292-72-6P 448292-75-9P 448292-76-0P
448296-01-3P 448296-04-6P 448296-05-7P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of microbiocidal N-phenyl-N-[4-(4-pyridyl)-pyrimidin-2-yl]amines)

RN 448267-86-5 HCAPLUS

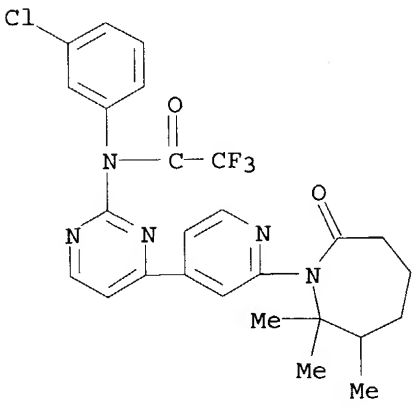
CN Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-N-[4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 448267-89-8 HCAPLUS
CN Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-N-[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

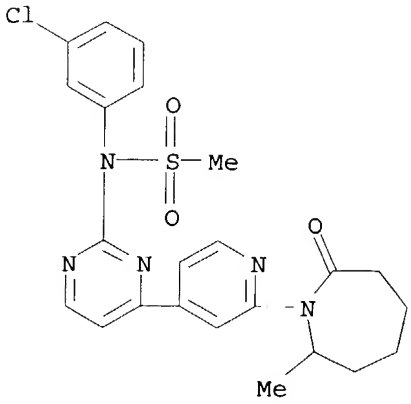


RN 448267-90-1 HCAPLUS
CN Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-N-[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

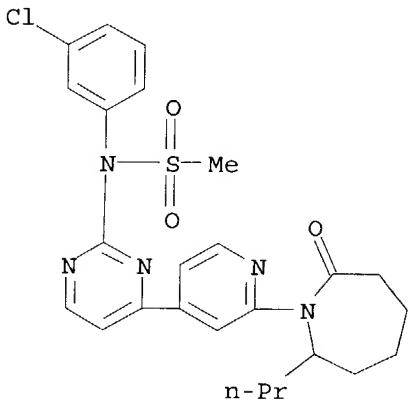


RN 448270-89-1 HCAPLUS
CN Methanesulfonamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-methyl-7-oxo-

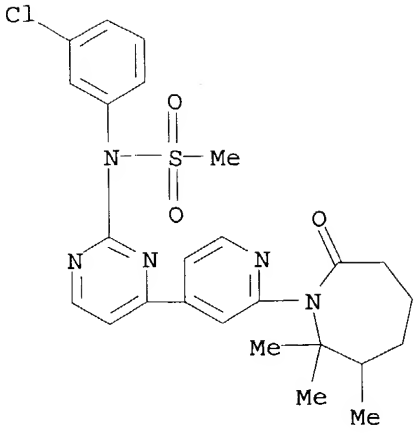
1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



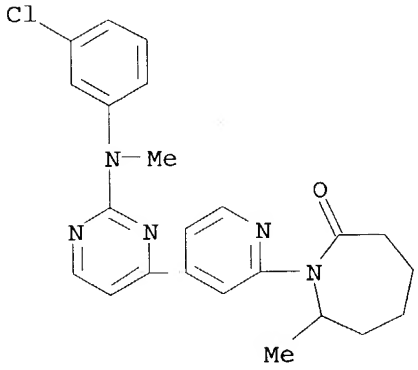
RN 448270-92-6 HCAPLUS
CN Methanesulfonamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



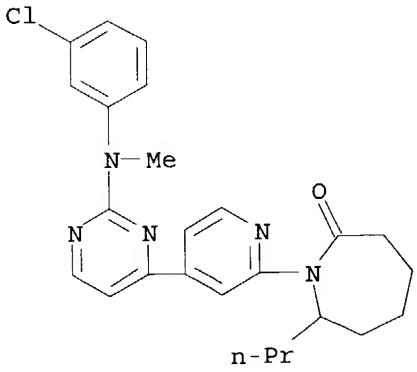
RN 448270-93-7 HCAPLUS
CN Methanesulfonamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 448274-18-8 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)methylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

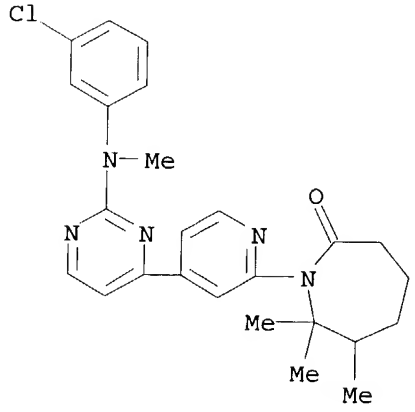


RN 448274-21-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)methylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)

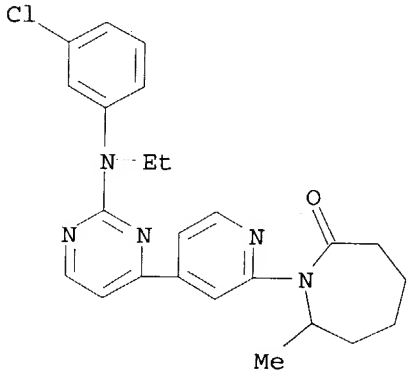


RN 448274-22-4 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)methylamino]-4-pyrimidinyl]-2-

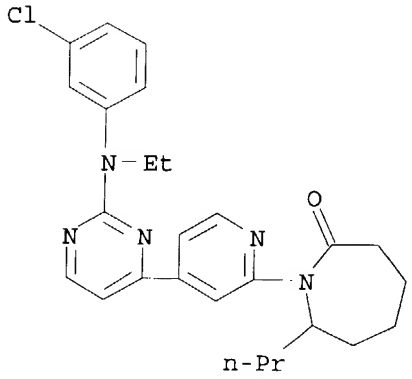
pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



RN 448277-11-0 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)ethylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

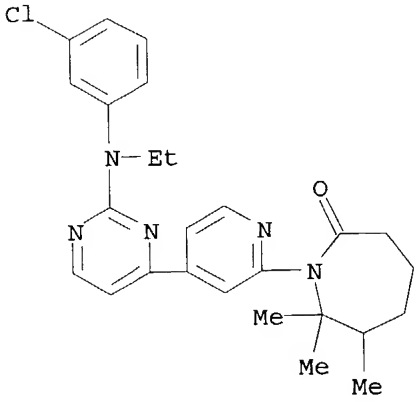


RN 448277-14-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)ethylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)

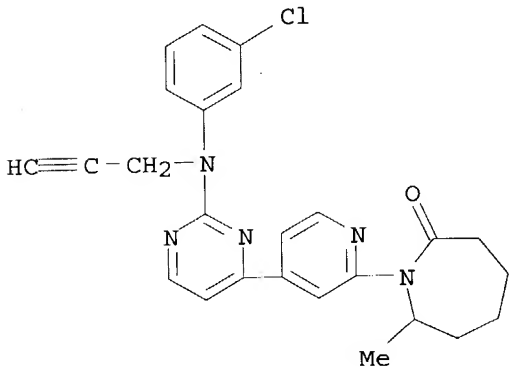


RN 448277-15-4 HCAPLUS

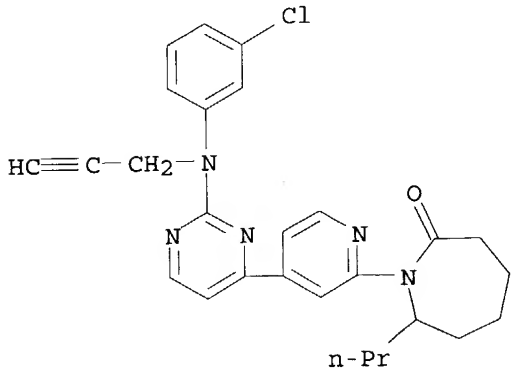
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)ethylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



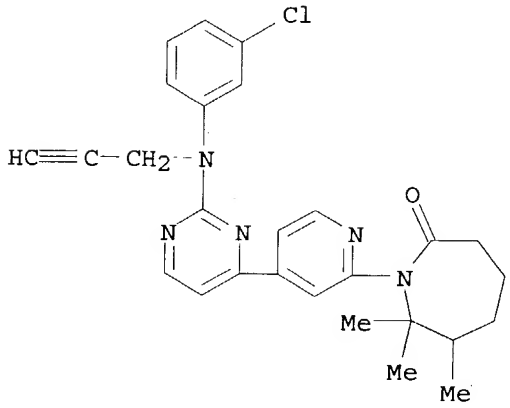
RN 448280-06-6 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)-2-propynylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



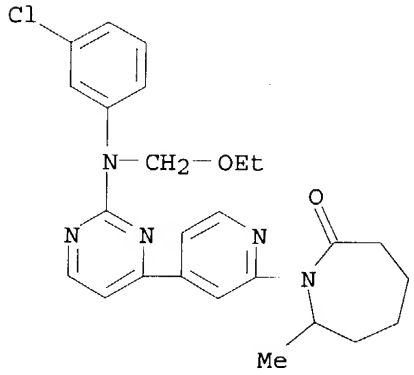
RN 448280-09-9 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)-2-propynylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



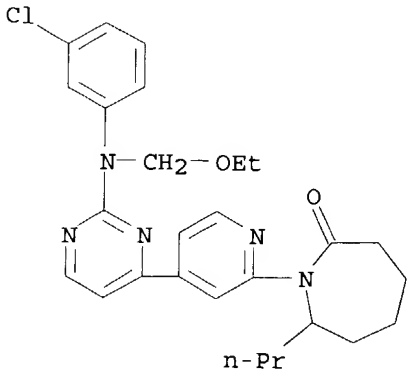
RN 448280-10-2 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)-2-propynylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



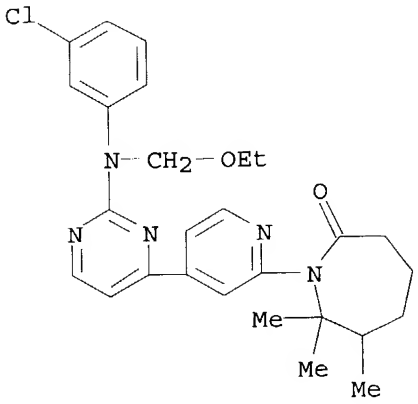
RN 448283-17-8 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(ethoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



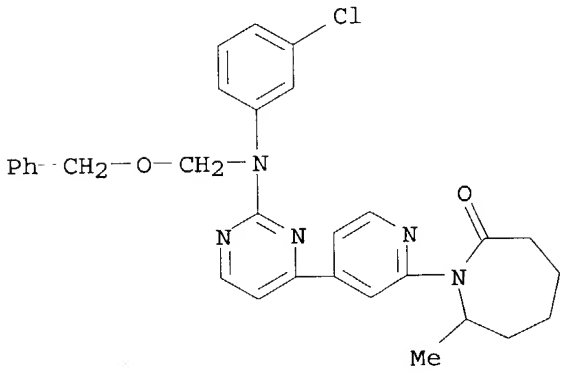
RN 448283-20-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(ethoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



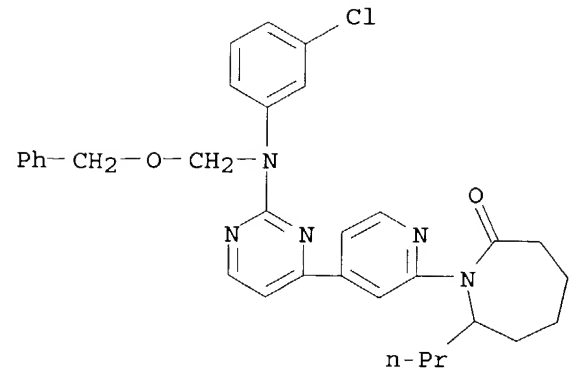
RN 448283-21-4 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(ethoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



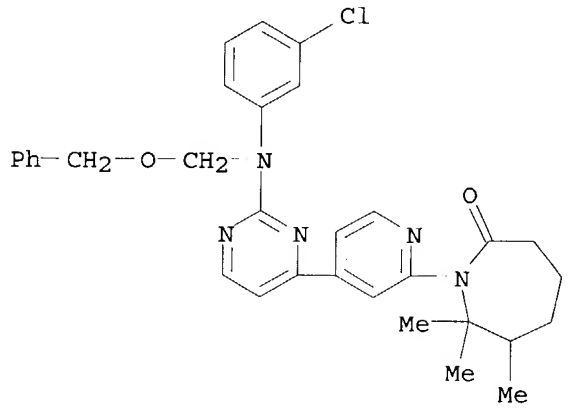
RN 448286-23-5 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(phenylmethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



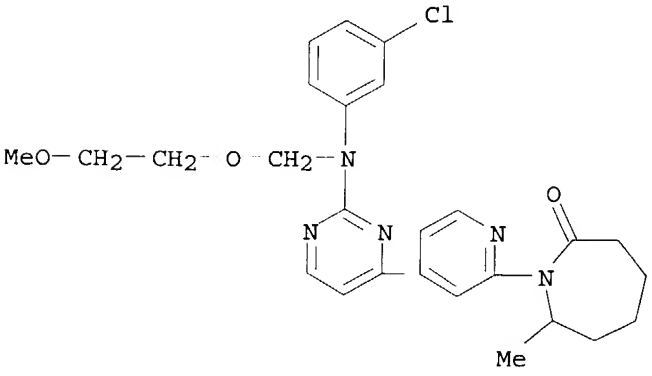
RN 448286-26-8 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(phenylmethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



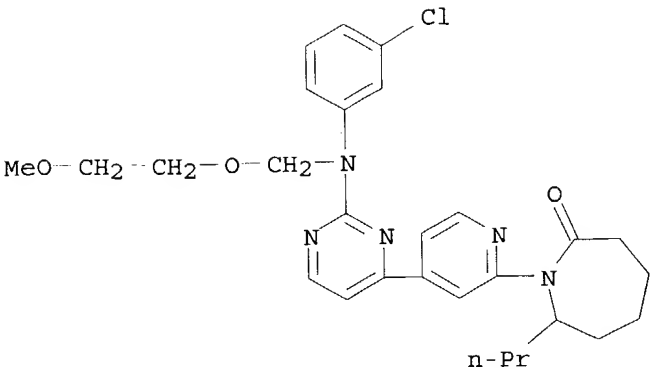
RN 448286-27-9 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(phenylmethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



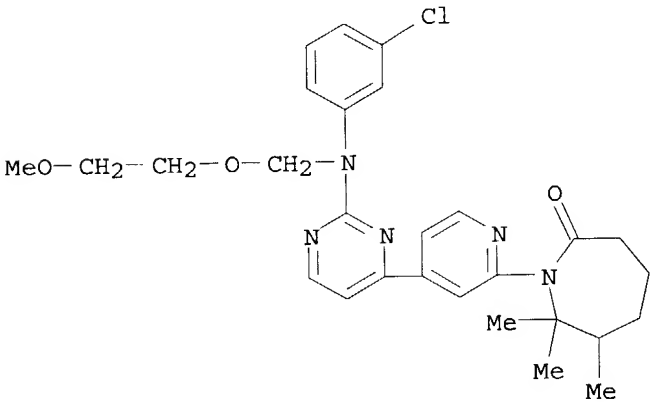
RN 448289-56-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(2-methoxyethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



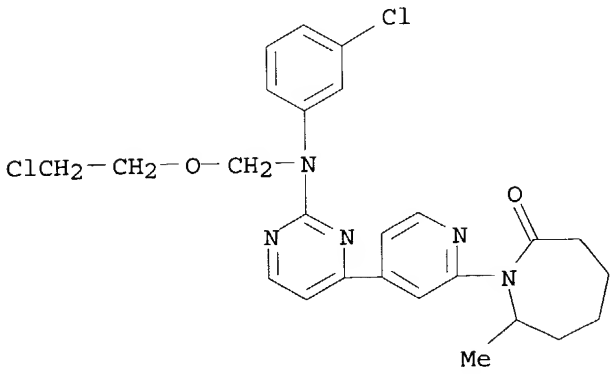
RN 448289-59-6 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(2-methoxyethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



RN 448289-60-9 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(2-methoxyethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)

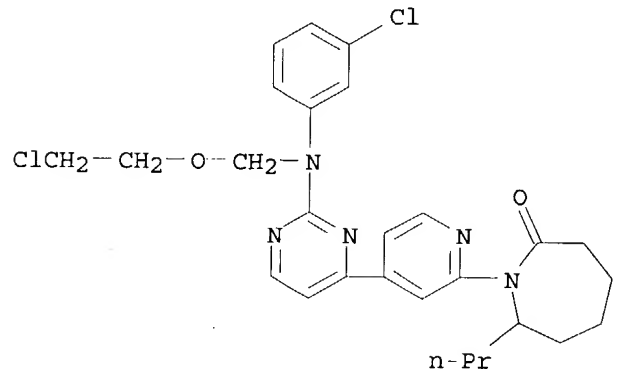


RN 448292-72-6 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[[(2-chloroethoxy)methyl](3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

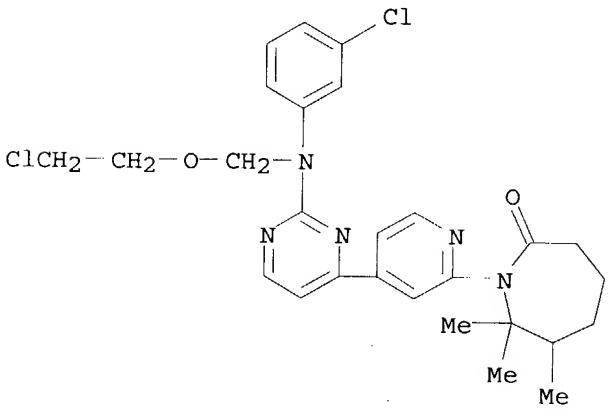


RN 448292-75-9 HCAPLUS

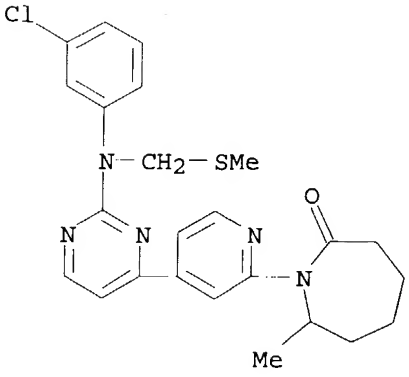
CN 2H-Azepin-2-one, 1-[4-[2-[[(2-chloroethoxy)methyl](3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



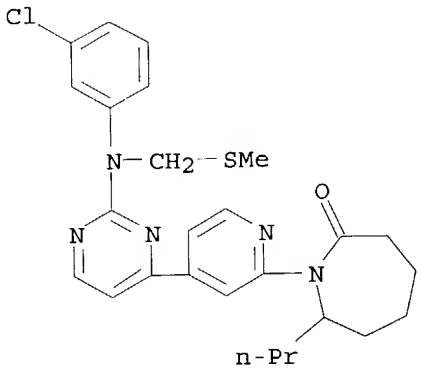
RN 448292-76-0 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[[(2-chloroethoxy)methyl](3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



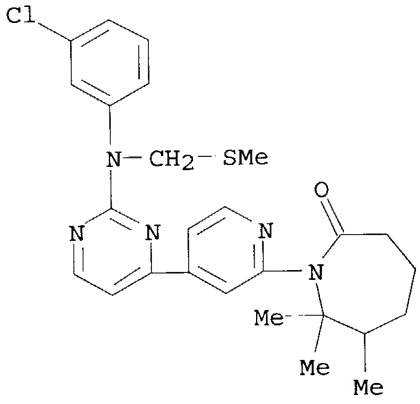
RN 448296-01-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(methylthio)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



RN 448296-04-6 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(methylthio)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



RN 448296-05-7 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(methylthio)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



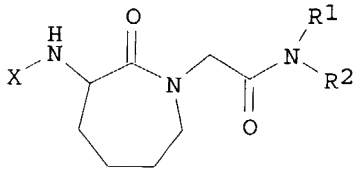
L95 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 5

ACCESSION NUMBER:	2002:103518 HCAPLUS
DOCUMENT NUMBER:	136:151180
TITLE:	Preparation of caprolactam compounds and their use as inhibitors of serine proteases
INVENTOR(S):	Bisacchi, Gregory S.; Seiler, Steven M.; Lawrence, R. Michael; Sutton, James C., Jr.; Slusarchyk, William A.; Zhao, Guohua
PATENT ASSIGNEE(S):	Bristol-Myers Squibb Company, USA
SOURCE:	U.S., 101 pp., Cont.-in-part of U.S. Ser. No. 478,632. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 6344450 B1 20020205 US 2000-633751 20000807
CA 2418995 AA 20020214 CA 2001-2418995 20010720
WO 2002012196 A2 20020214 WO 2001-US22829 20010720
WO 2002012196 A3 20030116
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2001080642 A5 20020218 AU 2001-80642 20010720
EP 1309609 A2 20030514 EP 2001-959048 20010720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004521071 T2 20040715 JP 2002-518174 20010720
PRIORITY APPLN. INFO.: US 1999-119374P P 19990209
US 2000-478632 A2 20000106
US 2000-633751 A 20000807
WO 2001-US22829 W 20010720
OTHER SOURCE(S): MARPAT 136:151180
GI



I

AB Caprolactam (azepan-2-one) derivs. [I; R1, R2 = H, each (un)substituted alkyl, alkenyl, alkynyl, aryl, aminoalkylaryl, aminocycloalkylalkyl, aminoalkyl, aminoalkylcycloalkyl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, polycycloalkylalkyl, cycloalkenyl, cycloheteroalkyl, cycloalkenylalkyl, polycycloalkenyl, or polycycloalkenylalkyl, or R1 and R2 can be taken with the nitrogen to which they are attached to form a cycloheteroalkyl ring; X = R4C(:Y), R3SO2 (wherein R3 is selected from optionally substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, polycycloalkylalkyl, etc.; Y = O, S; R4 = R5R6N, R7O, R8; wherein R5, R6 = each optionally substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, etc., or R5 and R6 can be taken with the nitrogen to which they are attached to form an optionally substituted cycloheteroalkyl ring; R7, R8 = each optionally substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, polycycloalkylalkyl, cycloalkenyl, etc.)] are prepared These compds. are inhibitors of factor Xa and tryptase (no data) and thus are useful as anticoagulants and in treating asthma, resp. Methods for treating (1) cardiovascular diseases associated with thrombosis, (2) thrombosis, coronary artery disease or cerebrovascular disease, associated with thrombosis, and (3) inflammation, asthma, or allergic rhinitis are also provided. The above cardiovascular diseases are atherosclerotic plaques, venous or arterial thrombosis, coagulation syndromes, ischemia and angina (stable and unstable), deep

vein thrombosis (DVT), disseminated intravascular coagulopathy, Kasabach-Merritt syndrome, pulmonary embolism, myocardial infarction, cerebral infarction, cerebral thrombosis, atrial fibrillation, cerebral embolism, thromboembolic complications of surgery, peripheral arterial occlusion, or restenosis following arterial injury induced by endogenous or exogenous events. A method for treating inflammatory bowel disease, psoriasis, conjunctivitis, atopic dermatitis, rheumatoid arthritis, osteoarthritis, chronic inflammatory joint disease, diseases of joint cartilage destruction, allergic rhinitis myocardial infarction, stroke, angina, treating or preventing diabetic retinopathy, fibrosis, scleroderma, pulmonary fibrosis, liver cirrhosis, myocardial fibrosis, neurofibromas, and hypertrophic scars is also provided. Thus, in an automated solution synthesis, a stock solution of 7 mg 4-[2-(methylamino)ethyl]pyridine in THF (300 μL), a stock solution of 8 mg diisopropylcarbodiimide in CH2Cl2 (300 μL), and a stock solution of 7-aza-1-hydroxybenzotriazole in DMF (300 μL), and a stock solution of 2-[(3S)-3-[N'-(3-methylphenyl)ureido]-2-oxoazepan-2-yl]acetic acid (preparation given) in CH2Cl2, were added via a liquid handler to a 16 mm + 100 mm tube and mixed in an orbital shaker for 72 h to give 2-[(3S)-3-[N'-(3-methylphenyl)ureido]-2-oxoazepan-2-yl]-N-methyl-N-[2-(4-pyridyl)ethyl]acetamide.

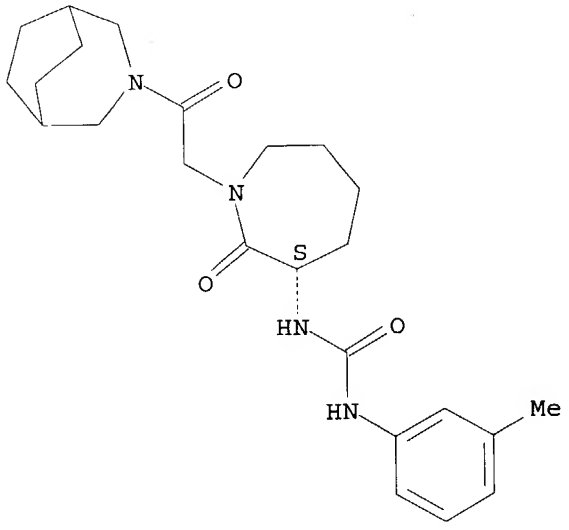
ED Entered STN: 07 Feb 2002

IT **288269-39-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactam compds. as inhibitors of serine proteases and factor Xa and anticoagulants for treating thrombosis-associated diseases, asthma, inflammation, or allergic rhinitis.)

RN 288269-39-6 HCAPLUS

CN 3-Azabicyclo[3.2.2]nonane, 3-[[(3S)-hexahydro-3-[[[(3-methylphenyl)amino]carbonyl]amino]-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

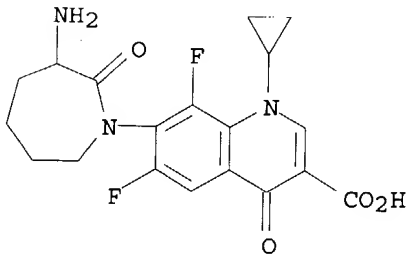


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 1995:38543 HCAPLUS
DOCUMENT NUMBER: 122:156098
TITLE: In vitro anti-Mycobacterium avium activities of quinolones: predicted active structures and mechanistic considerations
AUTHOR(S): Klopman, Gilles; Li, Ju-Yun; Wang, Shaomeng; Pearson, Anthony J.; Chang, Kieyoung; Jacobs, Michael R.; Bajaksouzian, Saralee; Ellner, Jerrold J.
CORPORATE SOURCE: Chem. Dept., Case Western Res. Univ., Cleveland, OH, 44106, USA
SOURCE: Antimicrobial Agents and Chemotherapy (1994), 38(8), 1794-1802
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English

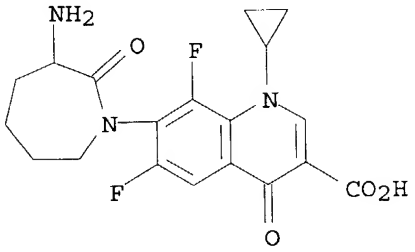
AB The relation between the structures of quinolones and their anti-M. avium activities has been previously derived by using the Multiple Computer-Automated Structure Evaluation program. A number of substructural constraints required to overcome the resistance of most of the strains have been identified. Nineteen new quinolones which qualify under these substructural requirements were identified by the program and subsequently tested. The substructural attributes identified by the program produced a successful a priori prediction of the anti-M. avium activities of the new quinolones. All 19 quinolones were active, and 4 of them are as active or better than ciprofloxacin. With these new quinolones, the updated multiple computer-automated structure evaluation program structure-activity relationship anal. has helped to uncover addnl. information about the nature of the substituents at the C5 and C7 positions needed for optimal inhibitory activity. A possible explanation of drug resistance based on the observation of suicide inactivation of bacterial cytochrome P 450 by the cyclopropylamine moiety has also been proposed and is discussed in this report. The view that the amount of the uncharged form present in a neutral pH solution plays a crucial role in the drug's penetration ability was confirmed.

ED Entered STN: 08 Nov 1994
IT **151895-29-3**, PD 130426
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(anti-Mycobacterium activity of)
RN 151895-29-3 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1995:2483 HCAPLUS
DOCUMENT NUMBER: 123:164953

TITLE: Anti-mycobacterium avium activity of quinolones: in vitro activities. [Erratum to document cited in CA120:27300f]
AUTHOR(S): Klopman, Gilles; Wang, Shaomeng; Jacobs, Michael R.; Bajaksouzian, Saralee; Edmonds, Kay; Ellner, Jerrold J.
CORPORATE SOURCE: Chem. Dep., Case West. Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Antimicrobial Agents and Chemotherapy (1993), 37(12), 2766
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstract or the index entries.
ED Entered STN: 08 Nov 1994
IT **151895-29-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Mycobacterium avium sensitivity to (Erratum))
RN 151895-29-3 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 8
ACCESSION NUMBER: 1994:27300 HCAPLUS
DOCUMENT NUMBER: 120:27300
TITLE: Anti-mycobacterium avium activity of quinolones: in vitro activities
AUTHOR(S): Klopman, Gilles; Wang, Shaomeng; Jacobs, Michael R.; Bajaksouzian, Saralee; Edmonds, Kay; Ellner, Jerrold J.
CORPORATE SOURCE: Chem. Dep., Case West. Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Antimicrobial Agents and Chemotherapy (1993), 37(9), 1799-806
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The MICs of 88 quinolones against 14 selected reference and clin. strains of Mycobacterium avium-M. intracellulare complex were determined Agents tested included ciprofloxacin, sparfloxacin (PD 131501), and 86 other exptl. quinolones. Test strains were selected to represent various susceptibilities to ciprofloxacin and other drug resistance profiles. MICs were determined by the microdilution method in 7HSF broth, with incubation for 14 days at 35°. The results showed 25 of the quinolones to be active against the strains, with MICs for 90% of the strains (MIC90s) of 2

to 32 μg/mL. Ten of these compds. had activities equivalent to or greater than that of ciprofloxacin. The most active compound was PD 125354, with an MIC50 of 0.5 μg/mL and an MIC90 of 2 μg/mL; comparable values for ciprofloxacin were 4 and 8 μg/mL, resp. The next most active compds., with MIC90s of 4 μg/mL, were sparfloxacin (PD 131501), PD 123982, PD 135144, and PD 119421. MIC90s of PD 131575, PD 126889, PD 122642, PD 139586, and PD 143289 were 8 μg/mL. Further evaluation of the most active agents is warranted, as is assessment of structure-activity relationships of active and inactive agents to elucidate the active portions of the compds. and to lead to the development of compds. with enhanced activity.

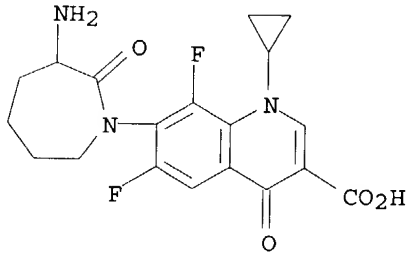
ED Entered STN: 22 Jan 1994

IT **151895-29-3**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Mycobacterium avium sensitivity to)

RN 151895-29-3 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 1992:530937 HCAPLUS

DOCUMENT NUMBER: 117:130937

TITLE: Derivatives of 1,2,3,4-tetrahydronaphthylamine endowed with nootropic activity and pharmaceutical compositions containing same

INVENTOR(S): Giannessi, Fabio; Ghirardi, Orlando; Misiti, Domenico; Tinti, Maria Ornella; Cozzolino, Roberto

PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite S.p.A., Italy

SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

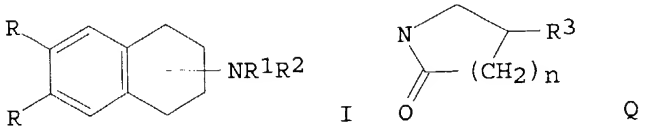
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 493346	A2	19920701	EP 1991-830574	19911219
EP 493346	A3	19920826		
EP 493346	B1	19950614		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
US 5192759	A	19930309	US 1991-809874	19911218
ES 2073725	T3	19950816	ES 1991-830574	19911219
JP 04275264	A2	19920930	JP 1991-338442	19911220

PRIORITY APPLN. INFO.: IT 1990-48605 A 19901221

OTHER SOURCE(S): MARPAT 117:130937
GI



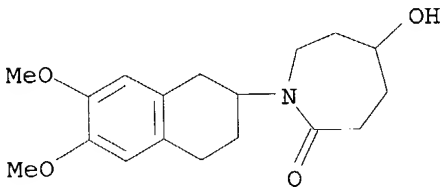
AB The title compds. I [R = H, OMe; NR1R2 is at the 1- or 2-position; R1 = H; R2 = L-prolyl, optionally substituted, L-pyroglutamyl, (pyrrolidin-2-on-1-yl)acetyl, 3-carboxy-2-hydroxypropyl; NR1R2 = Q (n = 1, 2, 3 and R3 = H, OH)] were prepared as nootropic agents. E.g., reaction of Z-L-proline and 1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthylamine in MeCN in the presence of EEDQ gave 85% product, which was hydrogenated in MeOH with 10% Pd/C at 40 psi for 2 h to give 71% N-(L-prolyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthylamine (II). Of the compds. prepared and tested, only II showed antiamnesic activity, without toxicity, in scopolamine- and electroconvulsive shock-induced amnesia.

ED Entered STN: 04 Oct 1992

IT **143254-67-5P 143254-69-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

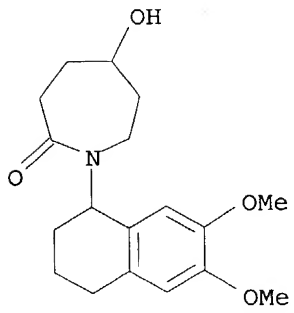
RN 143254-67-5 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 143254-69-7 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

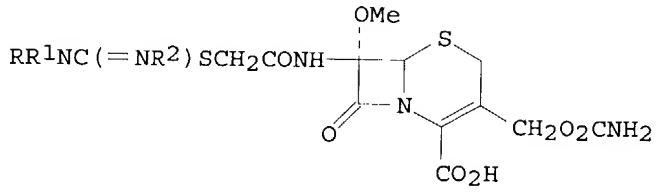


L95 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 1979:87491 HCAPLUS
DOCUMENT NUMBER: 90:87491
TITLE: 7-(Amidinothio)acetamido-7-methoxycephalosporins
INVENTOR(S): Czaja, Robert F.; Grabowski, Edward J. J.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4121041	A	19781017	US 1977-765477	19770204
PRIORITY APPLN. INFO.:			US 1977-765477	19770204

GI



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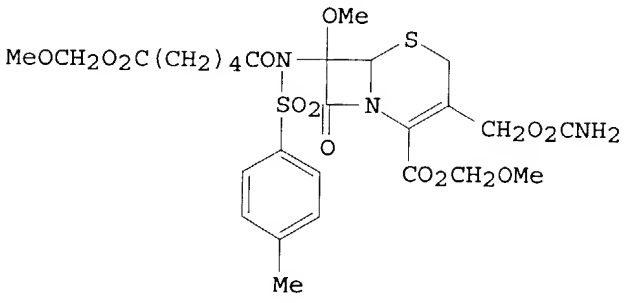


II

AB Cephalosporins I [R, R1,R2 = H, C1-5 alkyl, Ph; RR1 = (CH2)n (n = 3-6)] were prepared by treating RR1NCSNR2H with a 7-chloro- or 7-bromoacetamidocephem. Thus, II treated with ClCH2COCl gave the mono-Me ester which was saponified to give I (R - R2 = H).

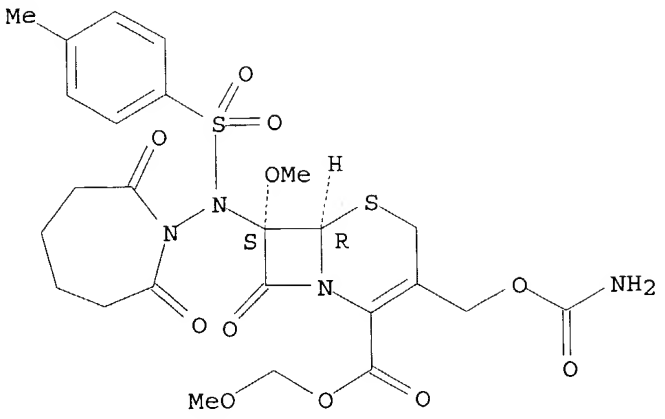
ED Entered STN: 12 May 1984

IT **69195-89-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloroacetyl chloride)

RN 69195-89-7 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(aminocarbonyl)oxy]methyl]-7-[(hexahydro-2,7-dioxo-1H-azepin-1-yl)[(4-methylphenyl)sulfonyl]amino]-7-methoxy-8-oxo-, methoxymethyl ester, (6R-cis)- (9CI) (CA INDEX NAME)

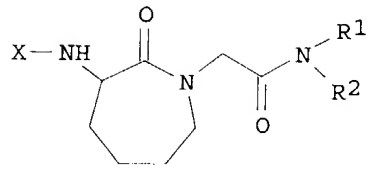
Absolute stereochemistry.



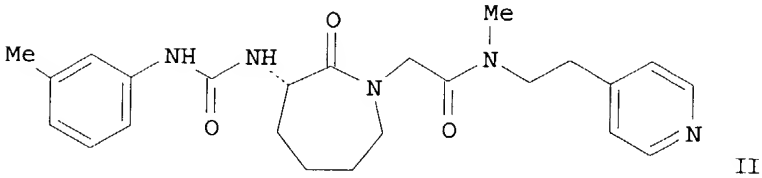
L95 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:573779 HCAPLUS
DOCUMENT NUMBER: 133:177117
TITLE: Preparation of lactam inhibitors of FXa
INVENTOR(S): Bisacchi, Gregory S.; Seiler, Steven M.; Lawrence, R. Michael
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000047563	A1	20000817	WO 2000-US1859	20000127
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2361919	AA	20000817	CA 2000-2361919	20000127
EP 1175405	A1	20020130	EP 2000-904564	20000127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AU 756174	B2	20030109	AU 2000-26300	20000127
PRIORITY APPLN. INFO.:			US 1999-119374P	P 19990209
			WO 2000-US1859	W 20000127

OTHER SOURCE(S): MARPAT 133:177117
GI



I



II

AB Lactam inhibitors of formula I [R1, R2 = alkyl, alkenyl, aryl, heteroaryl, cycloalkyl, etc.; R1R2 = cycloheteroalkyl; X = (substituted) CO, (substituted) CS, (substituted) SO2, etc.] are prepared These compds. are inhibitors of Factor Xa and thus are useful as anticoagulants (no data). A method for treating cardiovascular diseases associated with thromboses is also provided. Thus, II was prepared from 3-tert-butoxycarbonylaminohexahydro-2-azepinone, Et bromoacetate, m-tolylisocyanate and methylaminoethylpyridine.

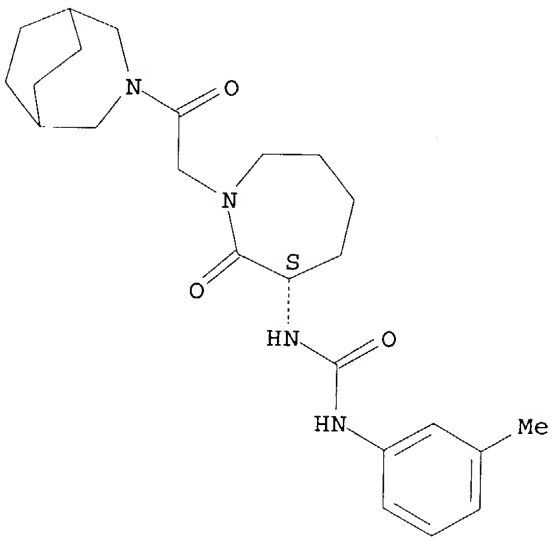
ED Entered STN: 18 Aug 2000

IT **288269-39-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactam inhibitors of Factor Xa)

RN 288269-39-6 HCAPLUS

CN 3-Azabicyclo[3.2.2]nonane, 3-[[(3S)-hexahydro-3-[[[(3-methylphenyl)amino]carbonyl]amino]-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

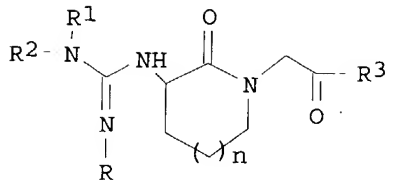


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:573666 HCAPLUS
DOCUMENT NUMBER: 133:164010
TITLE: Preparation of caprolactams, piperidinones, and pyrrolidinones as Factor Xa inhibitors in prevention or treatment of thromboses, coronary artery disease, or cerebrovascular disease in mammals
INVENTOR(S): Stein, Philip D.; Bisacchi, Gregory S.; Shi, Yan; O'Connor, Stephen P.; Li, Chi
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 284 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000047207	A1	20000817	WO 2000-US2883		20000202
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2360305	AA	20000817	CA 2000-2360305		20000202
US 6297233	B1	20011002	US 2000-496571		20000202
EP 1156803	A1	20011128	EP 2000-914505		20000202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
AU 760174	B2	20030508	AU 2000-35887		20000202
PRIORITY APPLN. INFO.:			US 1999-119372P	P	19990209
			US 1999-167428P	P	19991124
			WO 2000-US2883	W	20000202

OTHER SOURCE(S): MARPAT 133:164010
GI



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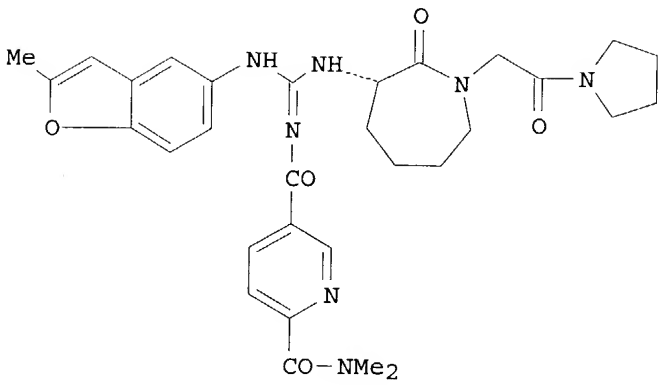


II

AB Title chiral compds. [I; R = CN, CONH2, COOCH2CH3, COC6H5, SO2NH2, OCH3, SO2N(CH3)2, SO2CH3, arylsulfonyl, heterocyclosulfonyl, (un)substituted Ph, heterocyclyl, heterocycleocarbonyl, alkoxylcarbonyl, arylaminocarbonyl; R1 = H, arylalkyl; R2 = alkyl, (un)substituted Ph, benzoheterocyclyl, cyclopentyl; R3 = heterocyclylamino, heterocyclyl, alkoxy, cycloalkylamino, OH; n = 0, 1, 2] , pharmaceutically acceptable salts, and stereoisomers are pred. as Factor Xa inhibitors and are useful as anticoagulants (no data). A method for treating cardiovascular diseases associated with thromboses is also provided. Thus, the title compound II was prepared

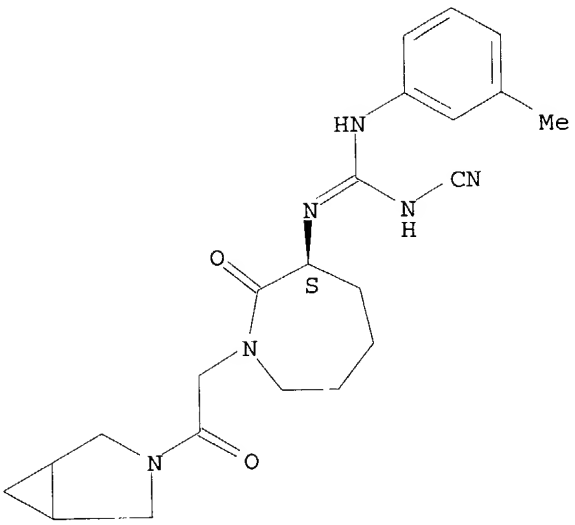
ED Entered STN: 18 Aug 2000

IT **288077-09-8P 288077-32-7P 288077-40-7P**
288081-29-8P 288081-35-6P 288081-83-4P
288082-97-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of caprolactams as Factor Xa inhibitors in prevention or treatment of thromboses, coronary artery disease, or cerebrovascular disease in mammals)

RN 288077-09-8 HCAPLUS

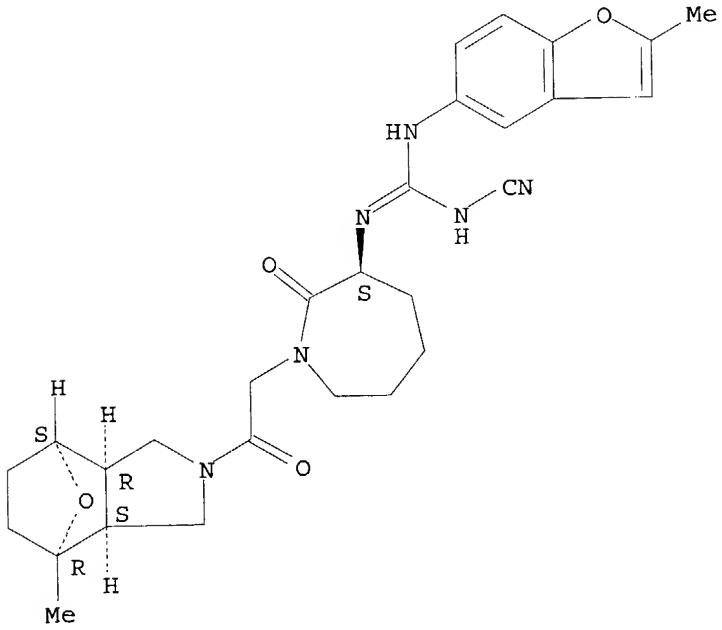
CN 3-Azabicyclo[3.1.0]hexane, 3-[[(3S)-3-[[(cyanoamino)[(3-methylphenyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



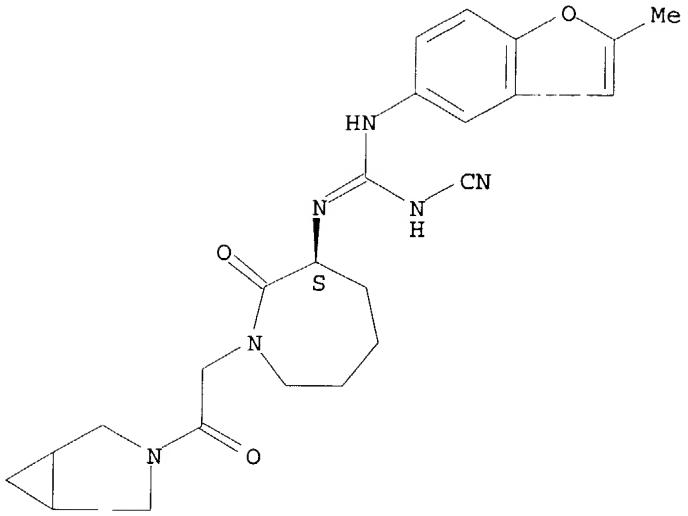
RN 288077-32-7 HCAPLUS
CN 4,7-Epoxy-1H-isoindole, 2-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-3-yl]acetyl]octahydro-4-methyl-, (3aS,4R,7S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



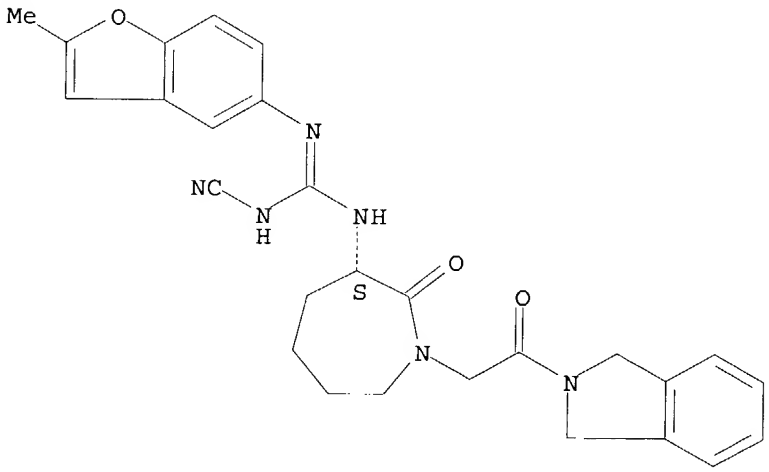
RN 288077-40-7 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane, 3-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



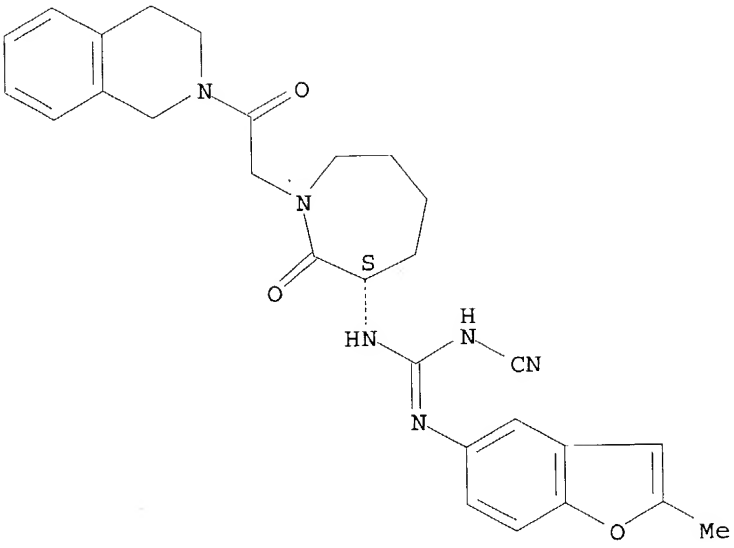
RN 288081-29-8 HCAPLUS
CN 1H-Isoindole, 2-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



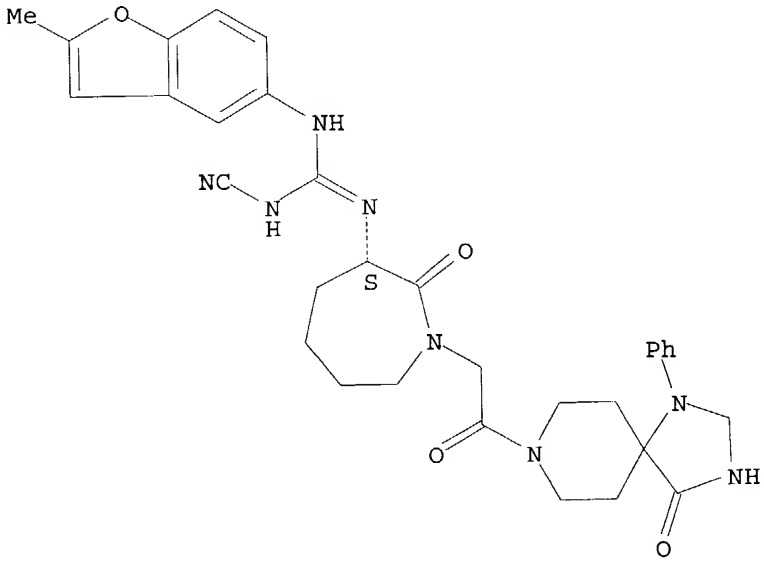
RN 288081-35-6 HCAPLUS
CN Isoquinoline, 2-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

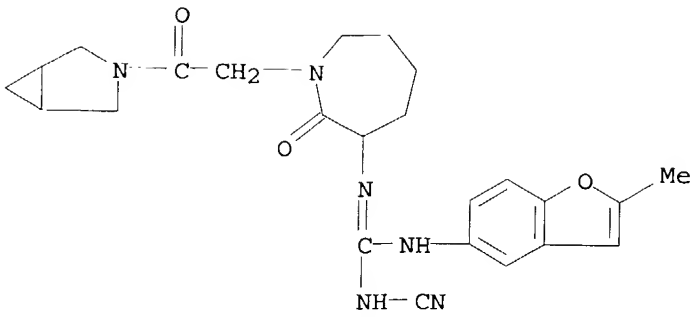


RN 288081-83-4 HCAPLUS
CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

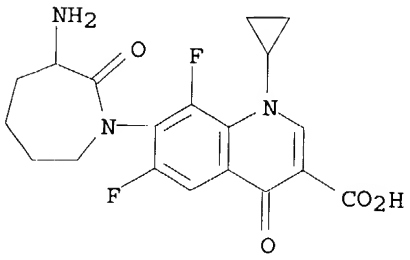


RN 288082-97-3 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane, 3-[[3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:409426 HCAPLUS
DOCUMENT NUMBER: 129:117473
TITLE: Activity of new quinolones against intracellular Mycobacterium avium in human monocytes. [Erratum to document cited in CA128:212700]
AUTHOR(S): Venkataprasad, Nandagopal; Jacobs, Michael R.; Johnson, John L.; Klopman, Gilles; Ellner, Jerrold J.
CORPORATE SOURCE: Division of Infectious Diseases, Case Western Reserve University, OH, 44106, USA
SOURCE: Journal of Antimicrobial Chemotherapy (1998), 41(6), 674
CODEN: JACHDX; ISSN: 0305-7453
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The ciprofloxacin MICs for strain PI 112/39 for inocula of 103, 104, and 105 were incorrectly reproduced in Table I; the corrected table is given.
ED Entered STN: 04 Jul 1998
IT **151895-29-3**, PD 130426
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(activity of new quinolones against intracellular Mycobacterium avium in human monocytes (Erratum))
RN 151895-29-3 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN

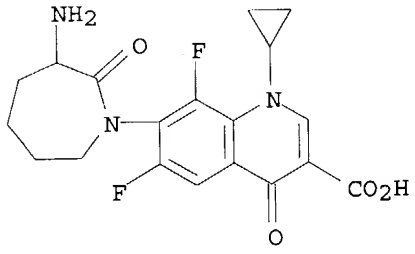
ACCESSION NUMBER: 1998:34271 HCAPLUS
DOCUMENT NUMBER: 128:212700
TITLE: Activity of new quinolones against intracellular Mycobacterium avium in human monocytes
AUTHOR(S): Venkataprasad, Nandagopal; Jacobs, Michael R.; Johnson, John L.; Klopman, Gilles; Ellner, Jerrold J.
CORPORATE SOURCE: Division of Infectious Diseases, Case Western Reserve University, OH, 44106, USA
SOURCE: Journal of Antimicrobial Chemotherapy (1997), 40(6), 841-845
CODEN: JACHDX; ISSN: 0305-7453
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ability to inhibit the in-vitro growth of mycobacteria within human monocytes is a useful screening assay for novel chemotherapeutic agents. In this study the MICs of a panel of new quinolones were determined by the broth microdilution method for two strains of Mycobacterium avium. Sixteen such compds. with MIC90s ranging from 2 to >32 mg/L were subsequently selected for the 7 day monocyte assay using ciprofloxacin for comparison. The degree of inhibition of intracellular growth correlated with the MICs. PD 139586, PD 143289, PD 135144, PD 119421 and PD 131575 were the most active new agents with activities superior to those of ciprofloxacin and sparfloxacin.

ED Entered STN: 21 Jan 1998

IT **151895-29-3**, PD 130426
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(activity of new quinolones against intracellular Mycobacterium avium in human monocytes)

RN 151895-29-3 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:288561 HCAPLUS
DOCUMENT NUMBER: 120:288561
TITLE: CO2 transfer by metal phenoxides: N-methyl-ε-caprolactam/sodium phenoxide as a selective reagent for carboxylation reactions
AUTHOR(S): Walther, D.; Ritter, U.; Gessler, S.; Sieler, J.; Kunert, M.
CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Friedrich-Schiller-Univ., Jena, Germany

SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (1994), 620(1), 101-6
CODEN: ZAACAB; ISSN: 0044-2313
DOCUMENT TYPE: Journal
LANGUAGE: German

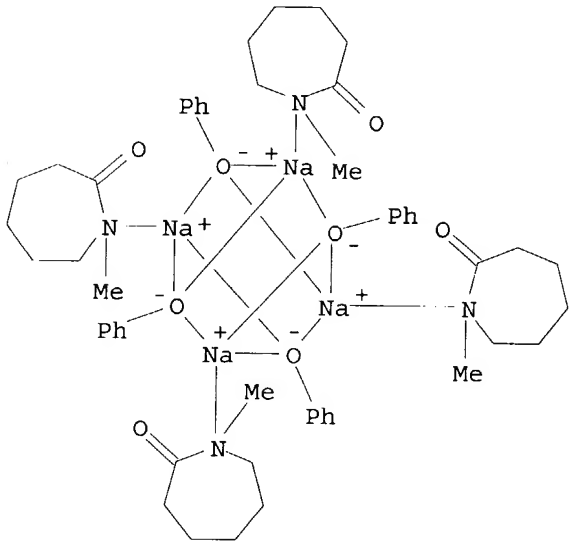
AB Carboxylation reactions of acetone and other substrates with active C-H bonds can be carried out selectively by complexes of NaOPh with N-methyl-ε-caprolactam (NMC) and CO2. With acetone 3-keto-glutaric acid is formed in 85% yield upon hydrolysis. X-ray structural anal. of [(NMC)Na(OPh)]4 shows that Na- and O ions of the phenoxide occupy the positions of a cube. NMC acts as monodentate ligand, the O atoms of the phenoxide are tridentate bridging ligands. The Li compound has a similar structure. The complex dissolved in NMC takes up 0.5 mol CO2 per mol Na which at room temperature and normal pressure is transferred to acetone.

ED Entered STN: 28 May 1994

IT **154935-77-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure and transfer agent in carboxylation of acetone)

RN 154935-77-0 HCAPLUS

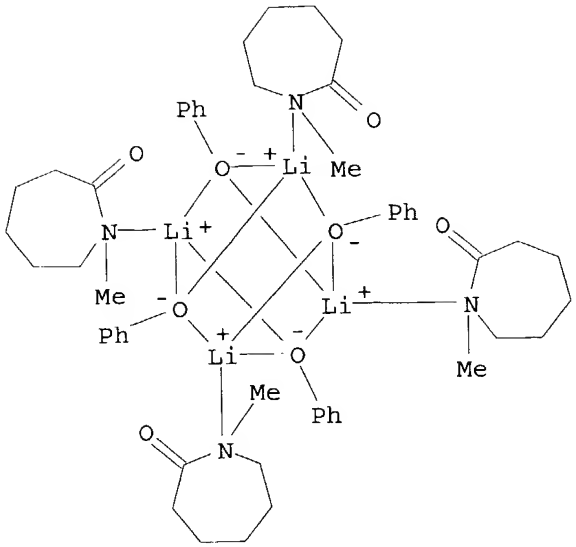
CN Sodium, tetrakis(hexahydro-1-methyl-2H-azepin-2-one-N1)tetra-μ3-phenoxytetra- (9CI) (CA INDEX NAME)



IT **154935-78-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 154935-78-1 HCAPLUS

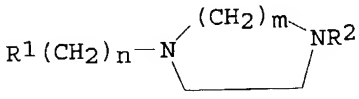
CN Lithium, tetrakis(hexahydro-1-methyl-2H-azepin-2-one-N1)tetra-μ3-phenoxytetra- (9CI) (CA INDEX NAME)



L95 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:77181 HCAPLUS
DOCUMENT NUMBER: 120:77181
TITLE: Preparation of hexahydroazepine derivatives as 5-HT1A serotoninergic receptor antagonists
INVENTOR(S): Takahashi, Nobuyuki; Suzuki, Yukio; Mochizuki, Daisuke; Tsujita, Ryuichi; Yaso, Masao; Komaki, Hisayuki
PATENT ASSIGNEE(S): Asahi Kasei Kogyo K. K., Japan
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9311116	A1	19930610	WO 1992-JP1533		19921124
W: CA, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
JP 05345764	A2	19931227	JP 1992-307377		19921117
PRIORITY APPLN. INFO.:			JP 1991-336053	A	19911126
			JP 1992-307377	A	19921117

OTHER SOURCE(S): CASREACT 120:77181; MARPAT 120:77181
GI



I

AB The title compds. [I; R1 = (un)substituted hexahydroazepin-1-yl; R2 = (un)substituted Ph, e.g., (trifluoromethyl)phenyl, (un)substituted pyridazinyl or 1,2-benzisothiazolyl; n = 2-5 integer; m = 2, 3], 5-HT1A

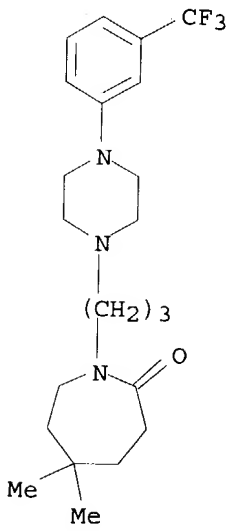
serotoninergic receptors and therefore useful for treatment of many ailments, e.g., anxiety, depression, motion sickness, hypertension (no data), are prepared E.g., caprolactam was treated with Cl-(CH2)3-Br in THF containing NaH at room temperature for 5 h to give 1-(3-chloropropyl)hexahydro-1H-azepine, which was refluxed with 1-[3-(trifluoromethyl)phenyl]piperazine in benzene containing Et3N for 139 h to give I [R1 = hexahydro-1H-azepin-1-yl, R2 = 3-(trifluoromethyl)phenyl, n = 3, m = 2], which had an affinity (Ki) of 13.7 nM for 5-HT1A receptors.

ED Entered STN: 19 Feb 1994

IT **151142-02-8P 151142-03-9P 151142-04-0P**
151142-05-1P 151142-06-2P 151142-07-3P
151142-08-4P 151142-09-5P 151142-10-8P
151142-11-9P 151142-17-5P 151142-18-6P
151142-19-7P 151142-20-0P 151142-21-1P
151142-22-2P 151142-23-3P 151142-24-4P
151142-25-5P 151142-26-6P 151142-27-7P
151142-54-0P 151142-72-2P 151142-73-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as serotoninergic receptor antagonist)

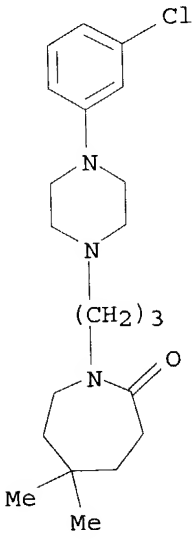
RN 151142-02-8 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

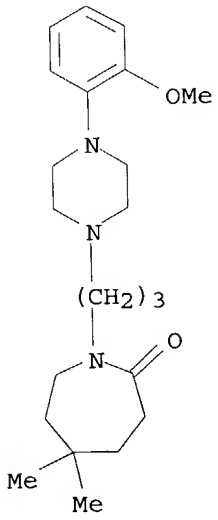


RN 151142-03-9 HCAPLUS

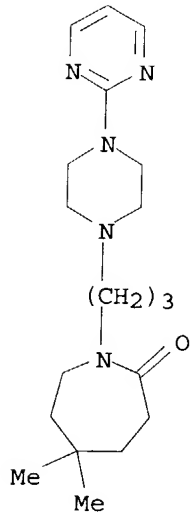
CN 2H-Azepin-2-one, 1-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



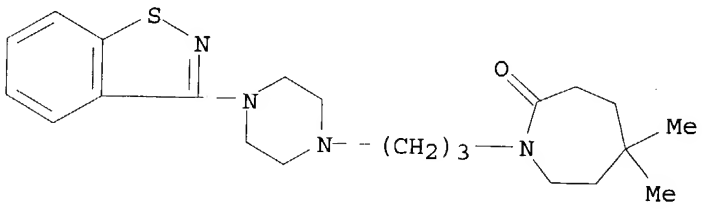
RN 151142-04-0 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-1-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-5,5-dimethyl- (9CI) (CA INDEX NAME)



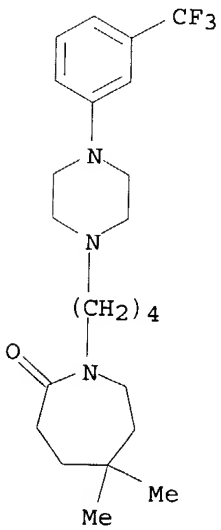
RN 151142-05-1 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



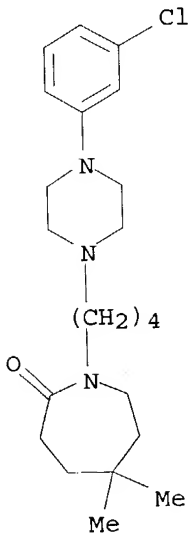
RN 151142-06-2 HCAPLUS
CN 2H-Azepin-2-one, 1-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



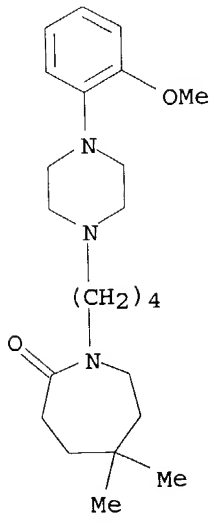
RN 151142-07-3 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



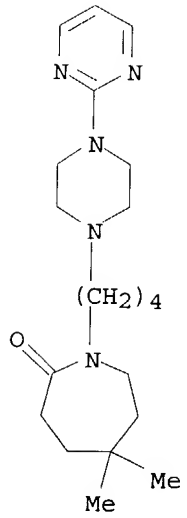
RN 151142-08-4 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



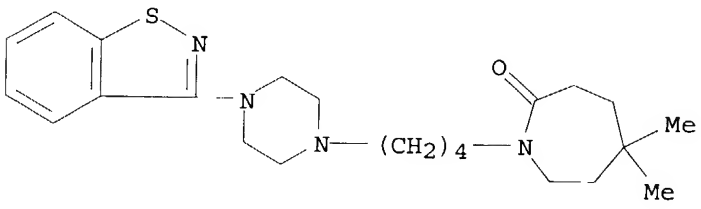
RN 151142-09-5 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-1-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-5,5-dimethyl- (9CI) (CA INDEX NAME)



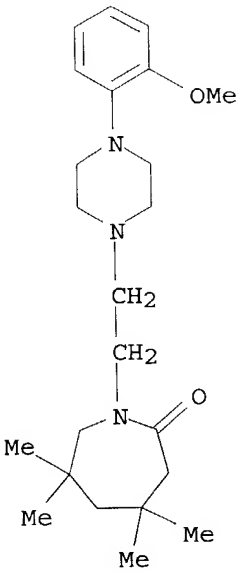
RN 151142-10-8 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[4-[4-(2-pyrimidinyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



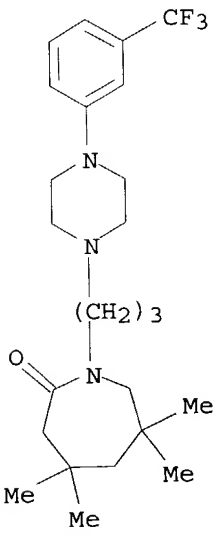
RN 151142-11-9 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



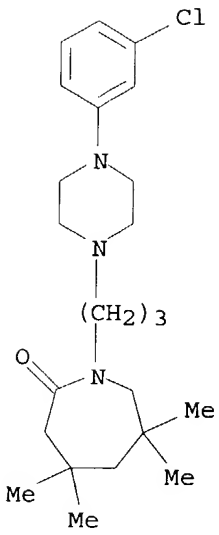
RN 151142-17-5 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-1-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



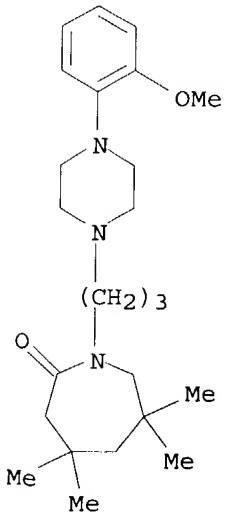
RN 151142-18-6 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



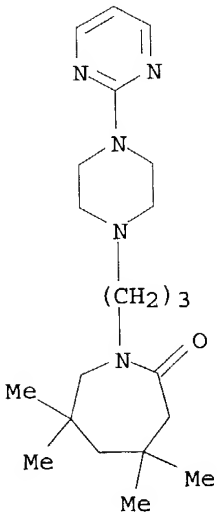
RN 151142-19-7 HCAPLUS
CN 2H-Azepin-2-one, 1-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



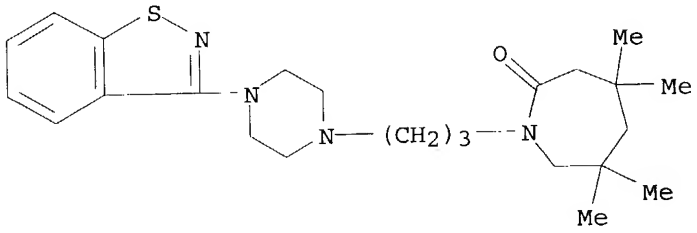
RN 151142-20-0 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-1-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



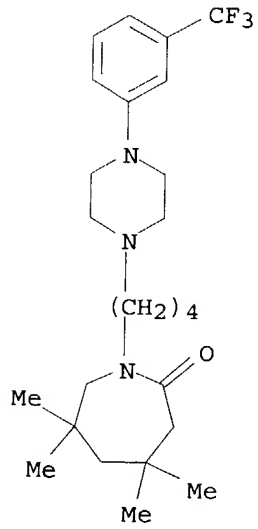
RN 151142-21-1 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



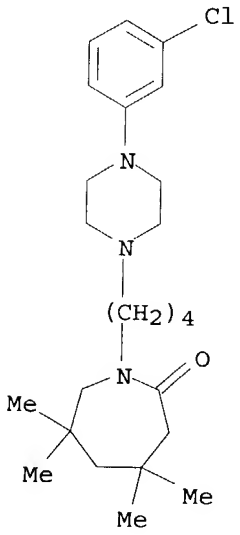
RN 151142-22-2 HCAPLUS
CN 2H-Azepin-2-one, 1-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



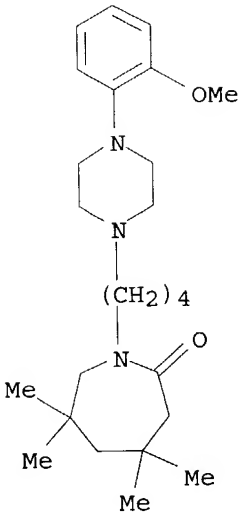
RN 151142-23-3 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



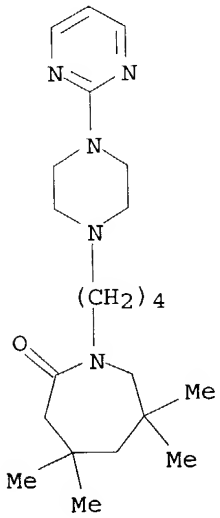
RN 151142-24-4 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



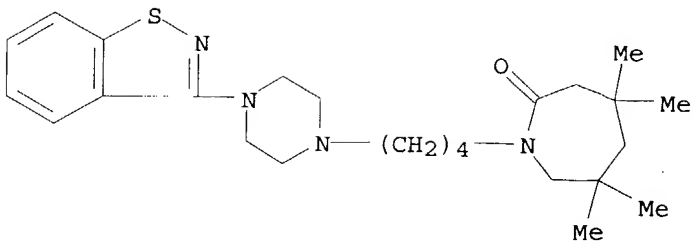
RN 151142-25-5 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-1-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



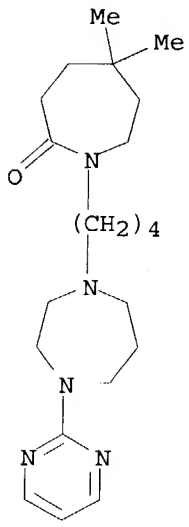
RN 151142-26-6 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[4-[4-(2-pyrimidinyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



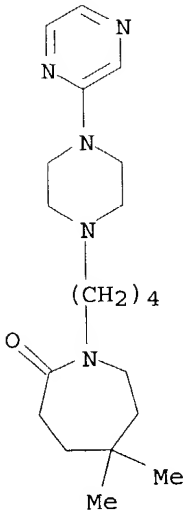
RN 151142-27-7 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



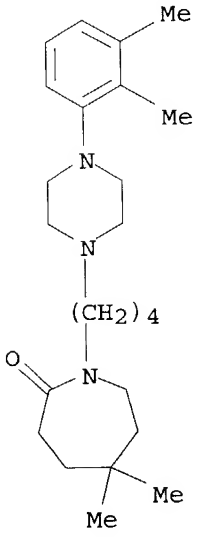
RN 151142-54-0 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[hexahydro-4-(2-pyrimidinyl)-1H-1,4-diazepin-1-yl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



RN 151142-72-2 HCAPLUS
CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[4-(4-pyrazinyl-1-piperazinyl)butyl]- (9CI) (CA INDEX NAME)



RN 151142-73-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[4-(2,3-dimethylphenyl)-1-piperazinyl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



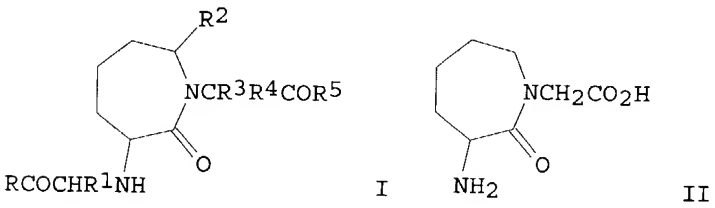
L95 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:217724 HCAPLUS
DOCUMENT NUMBER: 96:217724
TITLE: Substituted caprolactam derivatives as antihypertensives, pharmaceutical composition containing them, and intermediates
INVENTOR(S): Harris, Elbert E.; Patchett, Arthur A.; Thorsett, Eugene D.
PATENT ASSIGNEE(S): Merck and Co., Inc. , USA
SOURCE: Eur. Pat. Appl., 94 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 46291	A2	19820224	EP 1981-106372	19810817
EP 46291	A3	19820414		
EP 46291	B1	19851227		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DK 8103641	A	19820219	DK 1981-3641	19810817
ES 504791	A1	19830401	ES 1981-504791	19810817
JP 57112373	A2	19820713	JP 1981-128293	19810818
JP 02054342	B4	19901121		
NO 8103627	A	19830114	NO 1981-3627	19811027
FI 8103378	A	19830114	FI 1981-3378	19811028
ZA 8107685	A	19821027	ZA 1981-7685	19811106
US 4629787	A	19861216	US 1982-394749	19820702
ES 519057	A1	19840316	ES 1983-519057	19830117
US 4680392	A	19870714	US 1986-864234	19860519

PRIORITY APPLN. INFO.: US 1980-179305 A 19800818
US 1981-282580 A 19810713
US 1982-394749 A2 19820702

OTHER SOURCE(S): CASREACT 96:217724
GI



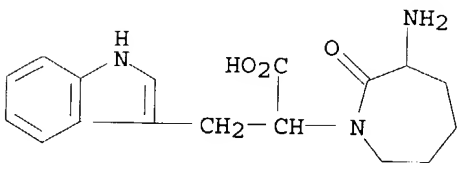
AB Antihypertensive (no data) caprolactams I [R, R5 = OH, (un)substituted alkoxy, aryloxy, amino; R1 = H, (un)substituted alkyl; R2 = H, (un)substituted alkyl, aryl, heteroaryl; R3 = H, (un)substituted alkyl, Ph; R4 = H, alkyl] were prepared Thus I (R = R5 = OH, R1 = CH2CH2Ph, R2-R4 = H) was prepared by reductive alkylation of the amine II with PhCH2CH2COCO2H. The amine was prepared from protected lysine in 4 steps.

ED Entered STN: 12 May 1984

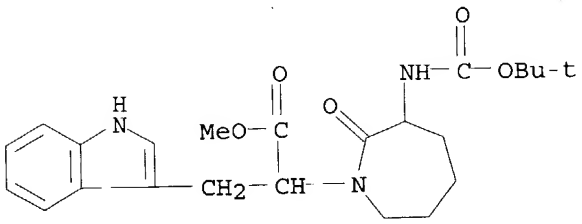
IT **81867-57-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of)

RN 81867-57-4 HCAPLUS

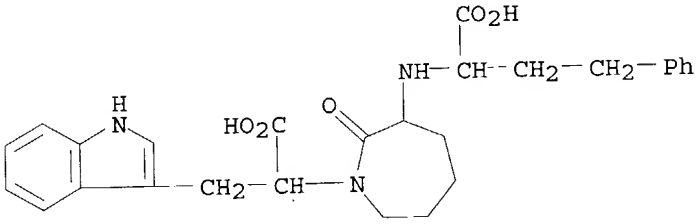
CN 1H-Indole-3-propanoic acid, α-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)- (9CI) (CA INDEX NAME)



IT **81867-56-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)
RN 81867-56-3 HCAPLUS
CN 1H-Indole-3-propanoic acid, α-[3-[[(1,1-dimethylethoxy)carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]-, methyl ester (9CI) (CA INDEX NAME)



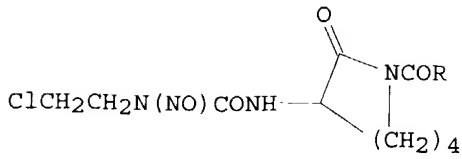
IT **81867-58-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 81867-58-5 HCAPLUS
CN 1H-Indole-3-propanoic acid, α-[3-[(1-carboxy-3-phenylpropyl)amino]hexahydro-2-oxo-1H-azepin-1-yl]- (9CI) (CA INDEX NAME)



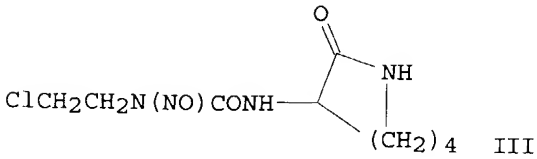
L95 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:443156 HCAPLUS
DOCUMENT NUMBER: 89:43156
TITLE: Nitrosourea derivatives
INVENTOR(S): Matsumoto, Jun; Murakami, Masuo; Sato, Noriaki; Hashimoto, Shinichi; Kawamura, Tsutomu; Ichikawa, Kaichiro
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53034790	A2	19780331	JP 1976-109628	19760913
			JP 1976-109628	19760913

PRIORITY APPLN. INFO.:
GI



I



III

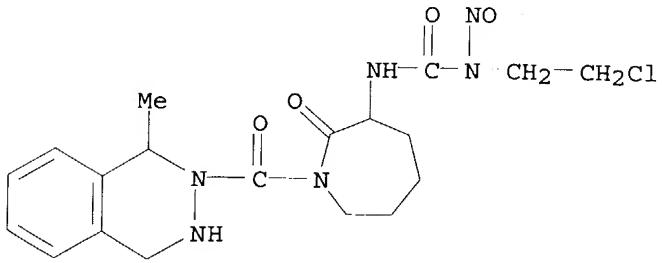
AB Nitrosourea derivs. I [R = 2-phenyl-2H-1,2,3-triazol-4-yl (II), 1-phenylpyrazol-5-yl, 4-methylphthalazan-3-yl, 1-adamantyl, 4-chloro-2-phenylpyrimidin-5-yl, Pr2NCO, 2,6-dioxopiperidin-4-ylmethyl, MeO2C] were prepared by silylation of III followed by reaction of RCOX (X = halo). I had antileukemic and anticarcinogenic activities (no data). Thus, 1.68 mL Et3N in dioxane was added to a mixture of 2.62 g III and 1.29 g Me3SiCl in dioxane, the whole stirred 20 h at room temperature, filtered, and the filtrate concentrated to give 10 mL solution; 2-phenyl-1,2,3-triazol-4-carbonyl chloride (1.5 g) in CH2Cl2 was added to 6 mL of the solution and the mixture stirred 3 days at room temperature to give 165 mg II.

ED Entered STN: 12 May 1984

IT **67060-43-9P 67060-44-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

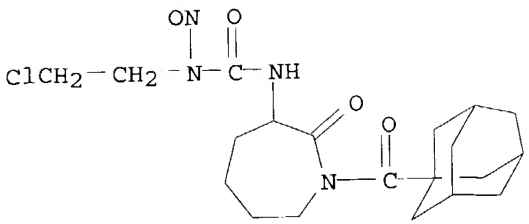
RN 67060-43-9 HCAPLUS

CN Phthalazine, 2-[[3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]carbonyl]-1,2,3,4-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



RN 67060-44-0 HCAPLUS

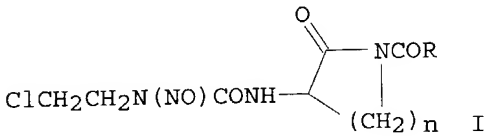
CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]hexahydro-1-(tricyclo[3.3.1.13,7]dec-1-ylcarbonyl)- (9CI) (CA INDEX NAME)



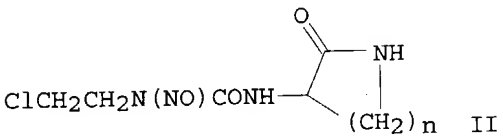
L95 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:6756 HCAPLUS
DOCUMENT NUMBER: 88:6756
TITLE: Nitroso urea derivatives
INVENTOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Atsushi; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52083747	A2	19770712	JP 1976-283	19760101
			JP 1976-283	19760101

PRIORITY APPLN. INFO.:
GI



I



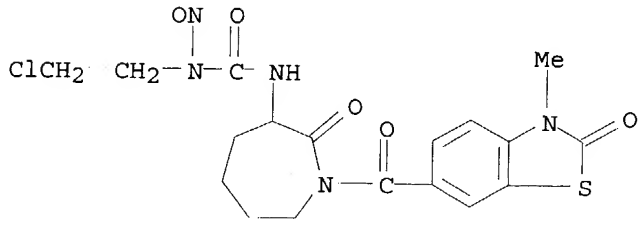
II

AB Twenty-eight title derivs. I [R = halo, substituted alkyl, (un)substituted alkenyl, (un)substituted aryl, (un)substituted heterocyclics; n = 2-10] were prepared by reaction of II with RCOX (X = halo). I had antitumor activity (some data given in mice). Thus, 174 mg 4-ClC6H4COCl in CHCl3 was added to 440 mg 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-nitrosourea mercuric salt in CHCl3 at room temperature and the mixture stirred 3 h to give 204 mg 1-(β-chloroethyl)-3-(N-p-chlorobenzoyl-2-oxo-3-hexahydroazepinyl)-1-nitrosourea.

ED Entered STN: 12 May 1984

IT **63847-31-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)

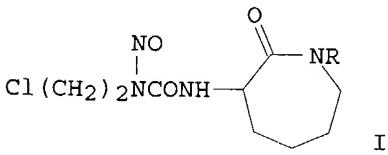
(preparation of)
RN 63847-31-4 HCAPLUS
CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]-1-[(2,3-dihydro-3-methyl-2-oxo-6-benzothiazolyl)carbonyl]hexahydro- (9CI) (CA INDEX NAME)



L95 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:535119 HCAPLUS
DOCUMENT NUMBER: 87:135119
TITLE: 1-(β-Chloroethyl)-3-substituted 1-nitrosoureas
INVENTOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52051363	A2	19770425	JP 1975-127807	19751023
PRIORITY APPLN. INFO.:			JP 1975-127807	19751023

GI



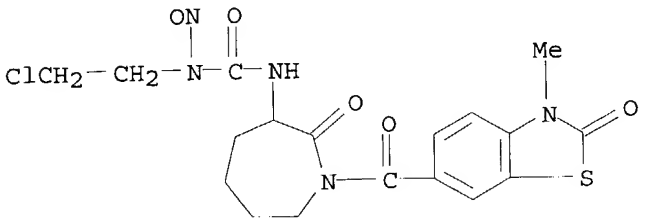
I

AB Thirteen title compds. (I, R = acyl) remedies for tumors, were prepared by treating non-substituted I with a silylating agent followed by acylation. Thus, 2.62 g 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-nitrosourea and Me3SiCl in dioxane were treated with NEt3 and treated with 352 mg p-[bis(β-chloroethyl)amino]benzoyl chloride in dichloromethane to give 403 mg I [R = p-[bis(β-chloroethyl)amino]benzoyl]. Among 12 I similarly prepared were (R given): 4-oxo-4H-thiopyran-3-carbonyl, p-O2NC6H4CO, p-(dimethylamino)benzoyl, 3-methyl-2-oxo-2,3-dihydrobenzothiazole-6-carbonyl.
ED Entered STN: 12 May 1984
IT **63847-31-4P 64148-23-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

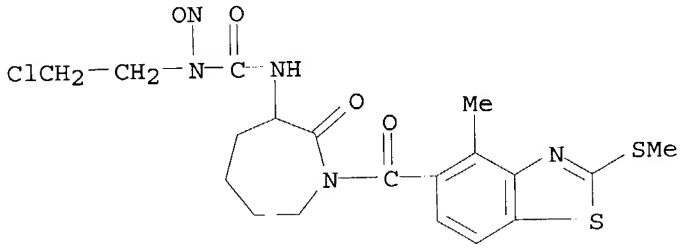
RN 63847-31-4 HCAPLUS

CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]-1-[(2,3-dihydro-3-methyl-2-oxo-6-benzothiazolyl)carbonyl]hexahydro- (9CI) (CA INDEX NAME)



RN 64148-23-8 HCAPLUS

CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]hexahydro-1-[[4-methyl-2-(methylthio)-5-benzothiazolyl]carbonyl]- (9CI) (CA INDEX NAME)



L95 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:502197 HCAPLUS

DOCUMENT NUMBER: 87:102197

TITLE: Nitrosourea derivatives

INVENTOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

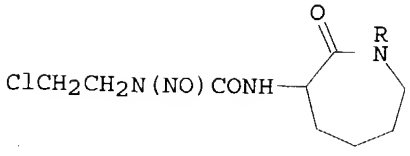
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52046072	A2	19770412	JP 1975-121967	19751008
			JP 1975-121967	19751008

PRIORITY APPLN. INFO.:

GI



I, R=R1CO

II, R=H

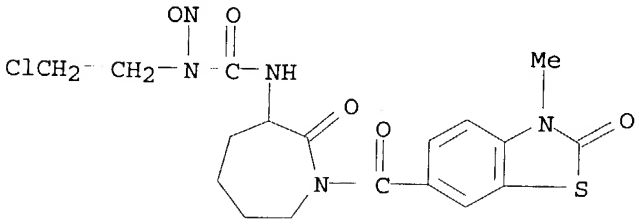
AB Fifteen nitrosourea derivs. I [R1 = (un)substituted Ph, furyl, pyrazinyl, H2C:CH, PhCH2, ClCH2, etc.] were prepared by reaction of II with R1COX (X = halo). I had anticancer activity (some data given in mice). Thus, 124 mg 4-ClC6H4COCl in CHCl3 was added to 440 mg II HgCl2 salt in CHCl3 and the mixture stirred 3 h at room temperature to give 204 mg I (R1 = 4-ClC6H4).

ED Entered STN: 12 May 1984

IT **63847-31-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anticarcinogenic activity of)

RN 63847-31-4 HCAPLUS

CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]-1-[(2,3-dihydro-3-methyl-2-oxo-6-benzothiazolyl)carbonyl]hexahydro- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 22-
YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y

L95 ANSWER 22 OF 30 USPATFULL on STN

ACCESSION NUMBER: 2004:83481 USPATFULL

TITLE: Microbiocidal n-phenyl-n-[4-(4-pyridyl-2-pyrimidin-2-yl]-amine derivatives

INVENTOR(S): Eberle, Martin, Basel, SWITZERLAND
Ziegler, Hugo, Basel, SWITZERLAND
Cederbaum, Fredrik, Basel, SWITZERLAND
Ackermann, Peter, Basel, SWITZERLAND
Schnyder, Anita, Basel, SWITZERLAND

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2004063937	A1	20040401	
APPLICATION INFO.:	US 2003-451930	A1	20030625	(10)
	WO 2001-IB2821		20011220	

	NUMBER	DATE
PRIORITY INFORMATION:	GB 2001-102	20010103

DOCUMENT TYPE: Utility

searched by D. Arnold 571-272-2532

FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: SYNGENTA CROP PROTECTION , INC., PATENT AND TRADEMARK DEPARTMENT, 410 SWING ROAD, GREENSBORO, NC, 27409

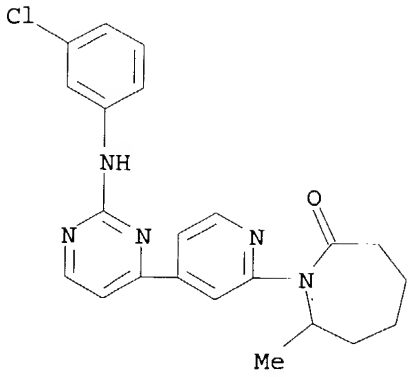
NUMBER OF CLAIMS: 15
EXEMPLARY CLAIM: 1
LINE COUNT: 1761
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel N-phenyl-4-(4-pyridyl)-2-pyrimidineamine derivatives of the general formula (1) wherein the sum of (m+p) together is 0, 1, 2 or 3; n and q are independently of each other 0 or 1, and the sum of (m+p+q) together is 1, 2, 3 or 4; R.sub.1 is hydrogen, halogen, alkoxy, haloalkyl, haloalkoxy or alkyl; R.sub.2 is hydrogen, C.sub.1-C.sub.6-alkyl, C.sub.1-C.sub.6-haloalkyl or C.sub.1-C.sub.6-alkoxy; R.sub.2A is hydrogen, C.sub.1-C.sub.6-alkyl, C.sub.3-C.sub.4-alkenyl or C.sub.3-C.sub.4-alkynyl; each of R.sub.3, R.sub.4, R.sub.5 and R.sub.6 is, independently of the others, hydrogen, C.sub.1-C.sub.6-alkyl, C.sub.1-C.sub.6-haloalkyl, hydroxy-C.sub.1-C.sub.6-alkyl or C.sub.1-C.sub.6-alkoxy-C.sub.1-C.sub.6-alkyl, or the ring members CR.sub.3R.sub.4 or CR.sub.5R.sub.6 or CR.sub.2R.sub.2A are independently of each other a carbonyl group (C.dbd.O) or a group C.dbd.S; X is C.dbd.O, C.dbd.S, S.dbd.O or O.dbd.S=O; Y is O, S, C.dbd.O, CH.sub.2A, --N(R.sub.8)--, --O--N(R.sub.8)--, --N(R.sub.8)--O-- or NH--; R.sub.7 is hydrogen, C.sub.1-C.sub.4-alkyl, C.sub.3-C.sub.4-alkenyl, C.sub.3-C.sub.4-alkynyl, --CH.sub.2OR.sub.8, CH.sub.2SR.sub.8, --C(O)R.sub.8, --C(O)OR.sub.8, SO2R.sub.8, SOR.sub.8 or SR.sub.8; and R.sub.8 is C.sub.1-C.sub.8-alkyl, C.sub.1-C.sub.8-alkoxyalkyl, C.sub.1-C.sub.8 haloalkyl or phenylC.sub.1-C.sub.2-alkyl wherein the phenyl may be substituted by up to three groups selected from halo or C.sub.1-C.sub.4-alkyl; or a salt thereof. The invention also relates to the preparation of the compounds and to agrochemical compositions comprising at least one of those compounds as active ingredient as well as the preparation of the said compositions and to the use of the compounds or of the compositions in controlling or preventing the infestation of plants by phytopathogenic microorganisms, especially fungi.

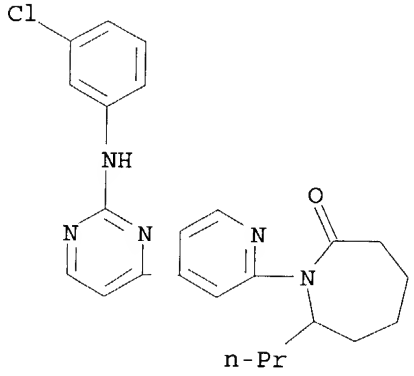
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **442164-61-6P 442164-64-9P 442164-65-0P**
442167-54-6P 442167-57-9P 442167-58-0P
442170-53-8P 442170-56-1P 442170-57-2P
442173-70-8P 442173-73-1P 442173-74-2P
442176-64-9P 442176-67-2P 442176-68-3P
442179-79-5P 442179-82-0P 442179-83-1P
442182-73-2P 442182-76-5P 442182-77-6P
442185-71-9P 442185-74-2P 442185-75-3P
442188-69-4P 442188-72-9P 442188-73-0P
442191-84-6P 442191-89-1P 442191-91-5P
(preparation of microbiocidal N-phenyl-N-[4-(4-pyridyl)-pyrimidin-2-yl]amines)

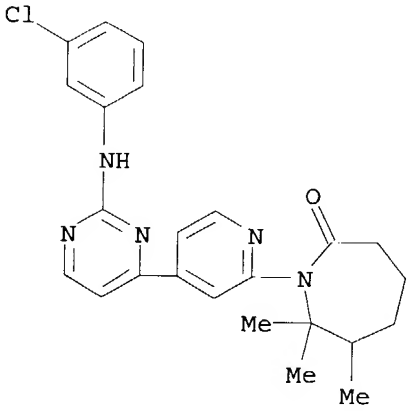
RN 442164-61-6 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



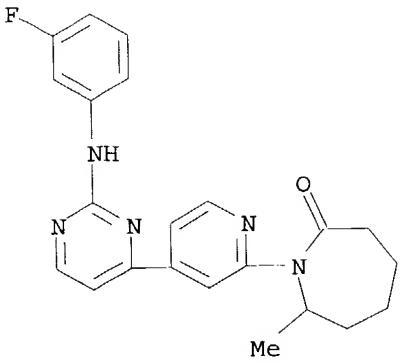
RN 442164-64-9 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



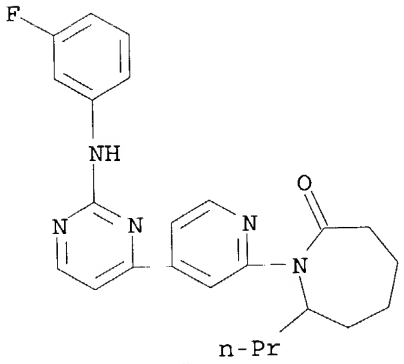
RN 442164-65-0 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



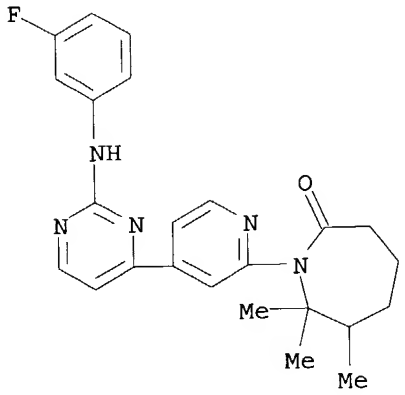
RN 442167-54-6 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



RN 442167-57-9 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)

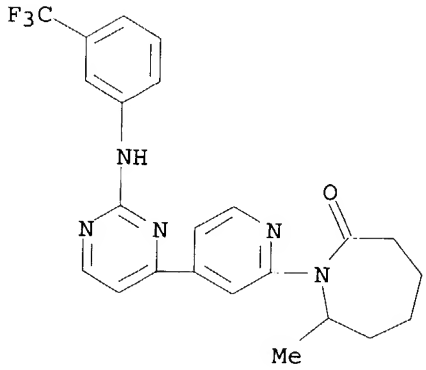


RN 442167-58-0 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)

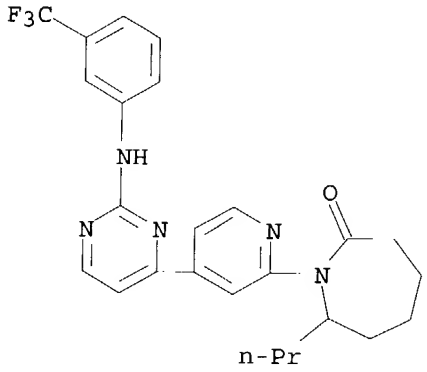


RN 442170-53-8 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[[3-

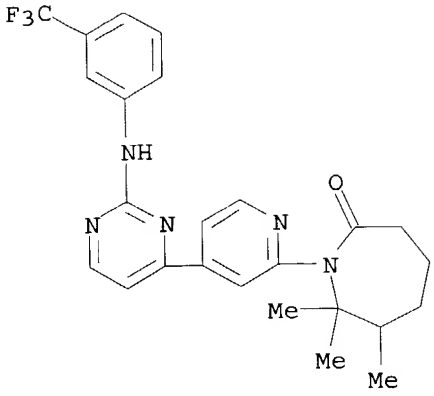
(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



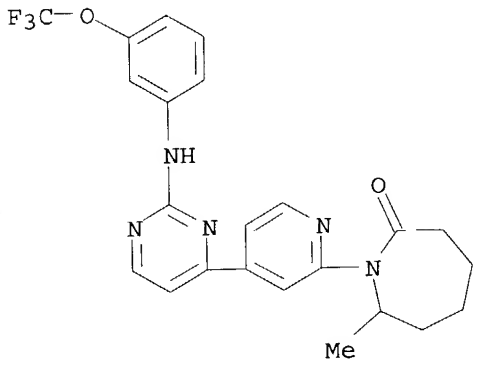
RN 442170-56-1 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-propyl-1-[4-[2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



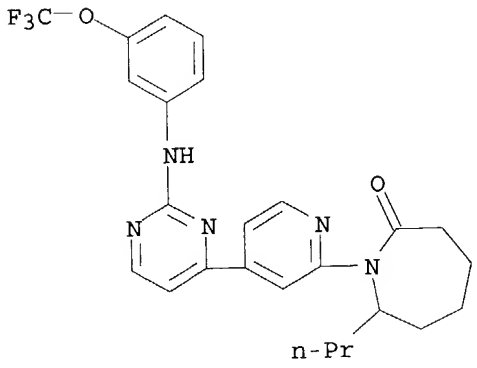
RN 442170-57-2 USPATFULL
CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 442173-70-8 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[[3-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

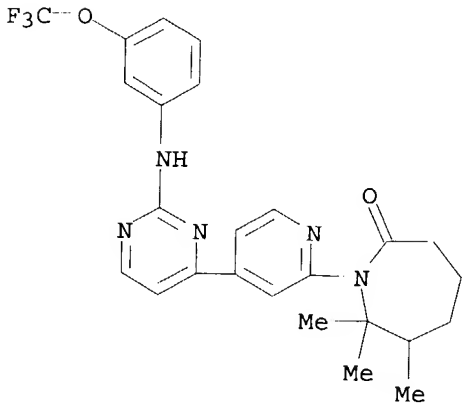


RN 442173-73-1 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-propyl-1-[4-[2-[[3-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

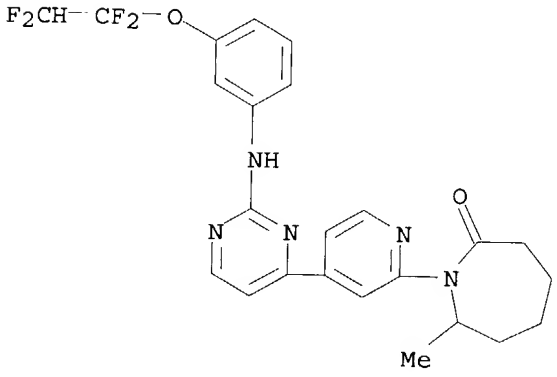


RN 442173-74-2 USPATFULL

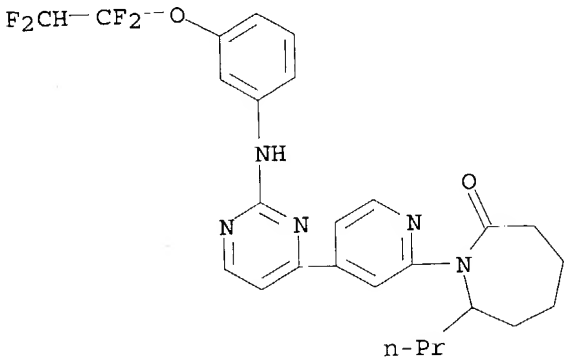
CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[[3-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



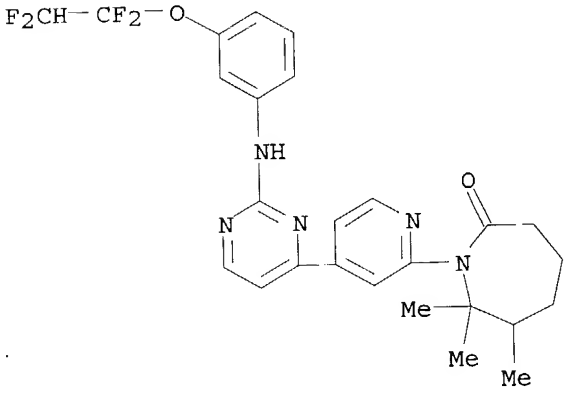
RN 442176-64-9 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[[3-(1,1,2,2-tetrafluoroethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



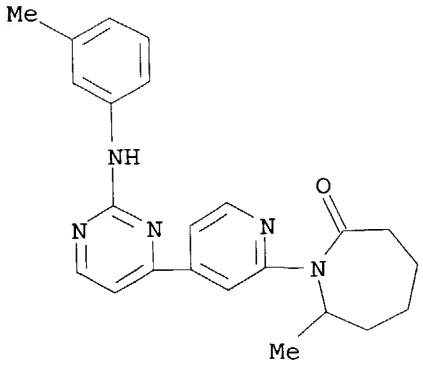
RN 442176-67-2 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-propyl-1-[4-[2-[[3-(1,1,2,2-tetrafluoroethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 442176-68-3 USPATFULL
CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[[3-(1,1,2,2-tetrafluoroethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

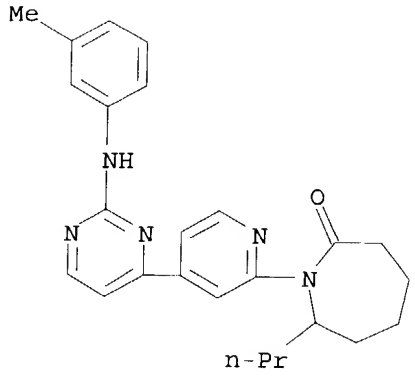


RN 442179-79-5 USPATFULL
CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[(3-methylphenyl)amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

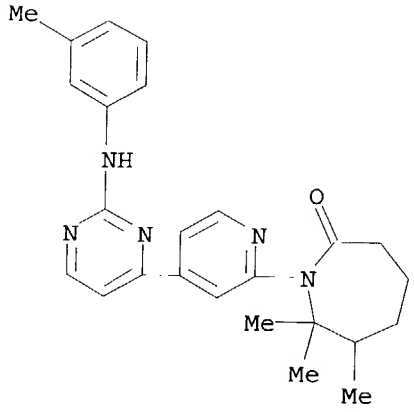


RN 442179-82-0 USPATFULL
CN 2H-Azepin-2-one, hexahydro-1-[4-[2-[(3-methylphenyl)amino]-4-pyrimidinyl]-

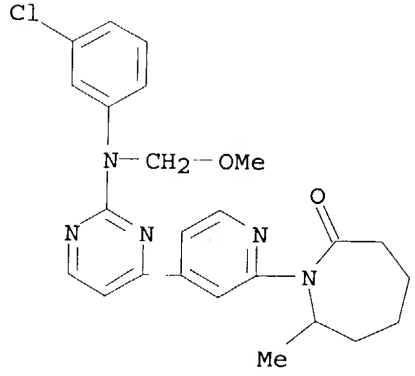
2-pyridinyl]-7-propyl- (9CI) (CA INDEX NAME)



RN 442179-83-1 USPATFULL
CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[(3-methylphenyl)amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

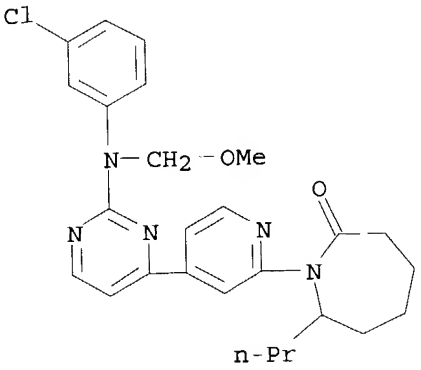


RN 442182-73-2 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(methoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

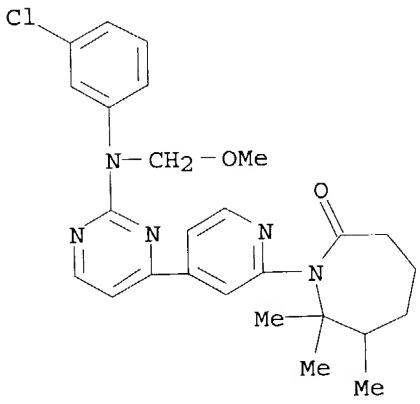


RN 442182-76-5 USPATFULL

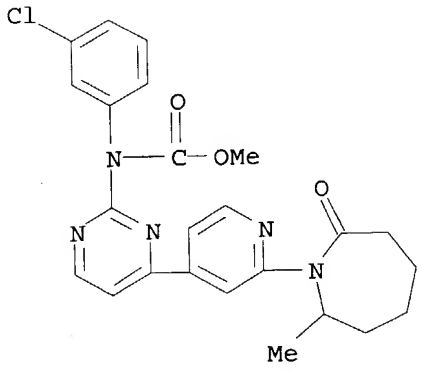
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(methoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



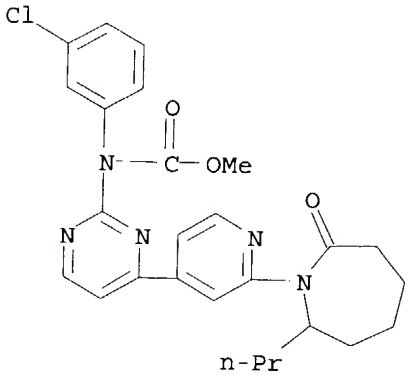
RN 442182-77-6 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(methoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



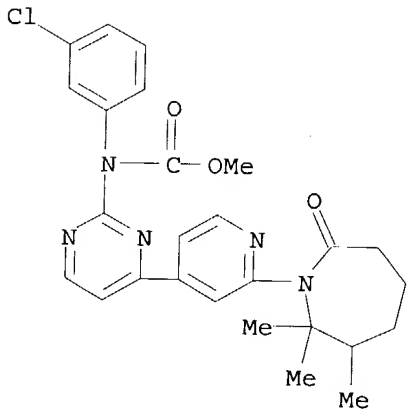
RN 442185-71-9 USPATFULL
CN Carbamic acid, (3-chlorophenyl)[4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)



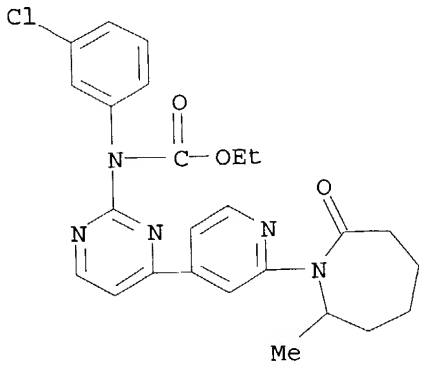
RN 442185-74-2 USPATFULL
CN Carbamic acid, (3-chlorophenyl)[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)



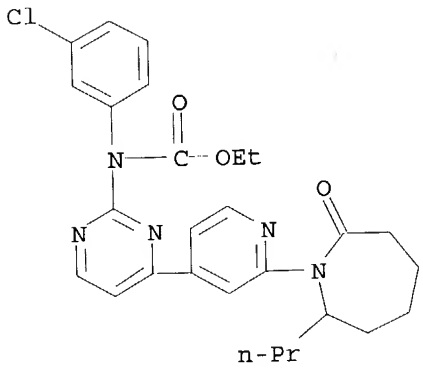
RN 442185-75-3 USPATFULL
CN Carbamic acid, (3-chlorophenyl)[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)



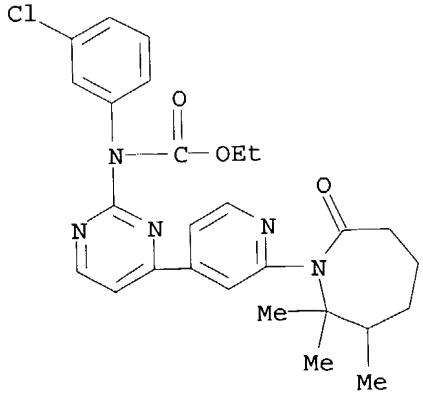
RN 442188-69-4 USPATFULL
CN Carbamic acid, (3-chlorophenyl)[4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 442188-72-9 USPATFULL
CN Carbamic acid, (3-chlorophenyl)[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

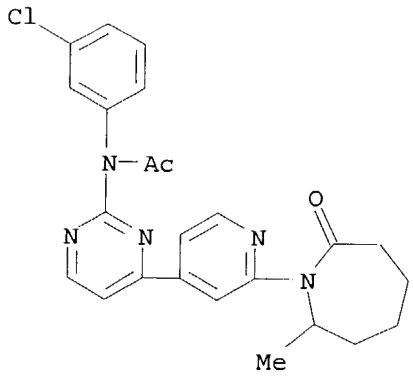


RN 442188-73-0 USPATFULL
CN Carbamic acid, (3-chlorophenyl)[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

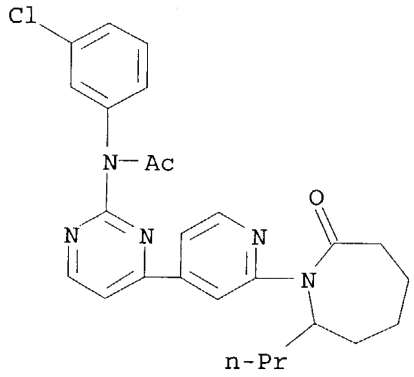


RN 442191-84-6 USPATFULL
CN Acetamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-

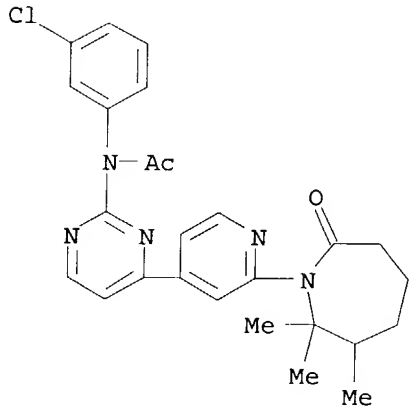
1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 442191-89-1 USPATFULL
CN Acetamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 442191-91-5 USPATFULL
CN Acetamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



L95 ANSWER 23 OF 30 USPATFULL on STN
ACCESSION NUMBER: 2001:168117 USPATFULL
TITLE: Lactam inhibitors of FXa and method
INVENTOR(S): Stein, Philip D., Pennington, NJ, United States
Bisacchi, Gregory S., Ringoes, NJ, United States
Shi, Yan, Flourtown, PA, United States
O'Connor, Stephen P., Lambertville, NJ, United States
Li, Chi, Randolph, NJ, United States
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, Princeton, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6297233	B1	20011002	
APPLICATION INFO.:	US 2000-496571		20000202	(9)

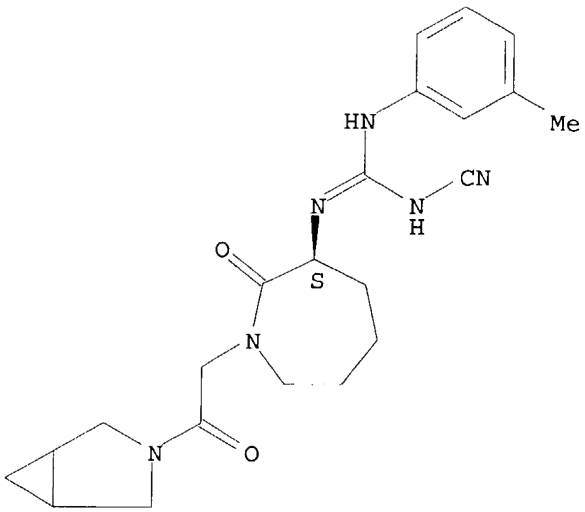
DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Kifle, Bruck
LEGAL REPRESENTATIVE: Rodney, Burton
NUMBER OF CLAIMS: 18
EXEMPLARY CLAIM: 1
LINE COUNT: 4323
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Caprolactam inhibitors are provided which have the structure ##STR1##

including pharmaceutically acceptable salts thereof and all stereoisomers thereof, and prodrugs thereof, wherein n is 1 to 5; and

and Y R.sup.1, R.sup.2, R.sup.3, R.sup.5, R.sup.5a, R.sup.6, R.sup.7, R.sup.8, R.sup.9 and R.sup.10 are as defined herein. These compounds are inhibitors of Factor Xa and thus are useful as anticoagulants. A method for treating cardiovascular diseases associated with thromboses is also provided.

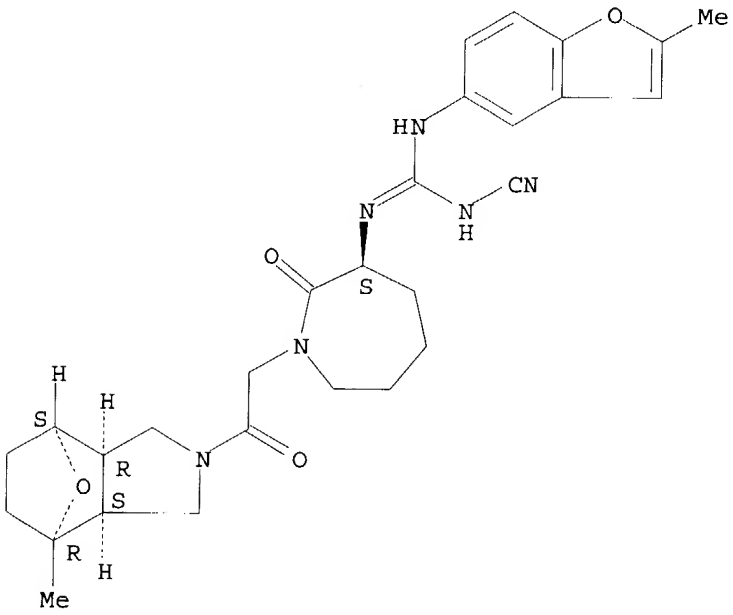
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **288077-09-8P 288077-32-7P 288077-40-7P**
288081-29-8P 288081-35-6P 288081-83-4P
288082-97-3P
(preparation of caprolactams as Factor Xa inhibitors in prevention or treatment of thromboses, coronary artery disease, or cerebrovascular disease in mammals)
RN 288077-09-8 USPATFULL
CN 3-Azabicyclo[3.1.0]hexane, 3-[[(3S)-3-[[(cyanoamino)[(3-methylphenyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



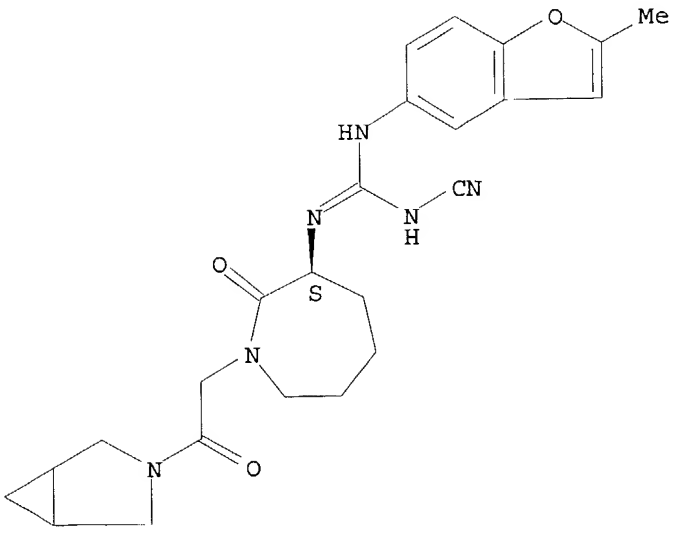
RN 288077-32-7 USPATFULL
CN 4,7-Epoxy-1H-isoindole, 2-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-3-yl]acetyl]octahydro-4-methyl-, (3aS,4R,7S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



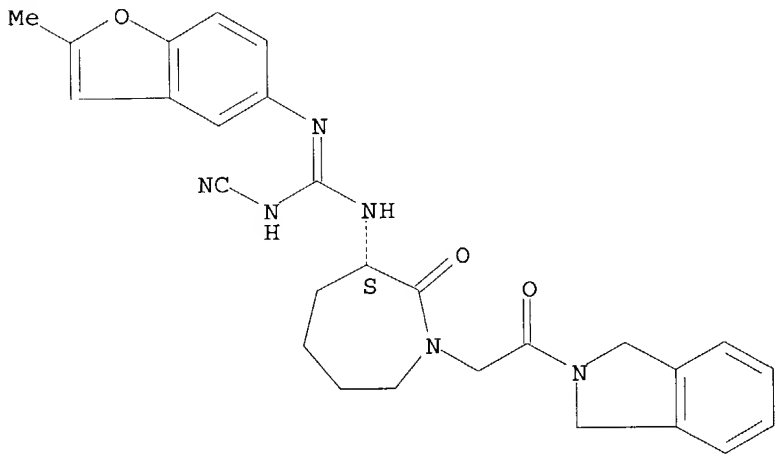
RN 288077-40-7 USPATFULL
CN 3-Azabicyclo[3.1.0]hexane, 3-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



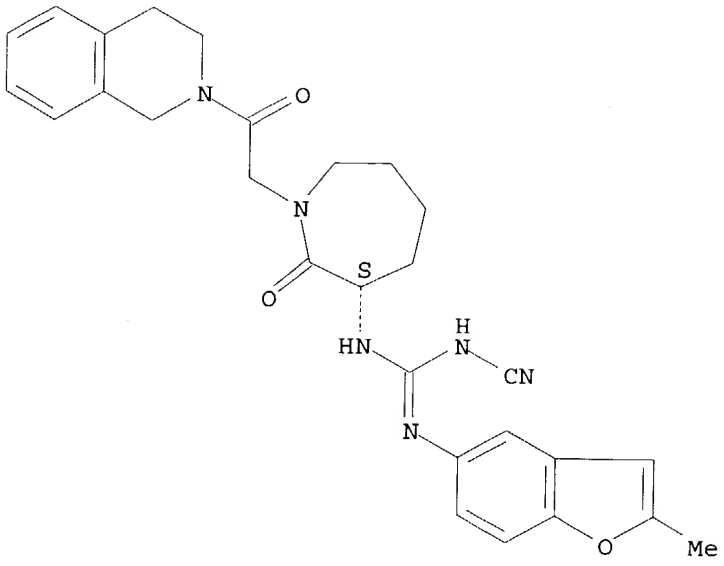
RN 288081-29-8 USPATFULL
CN 1H-Isoindole, 2-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



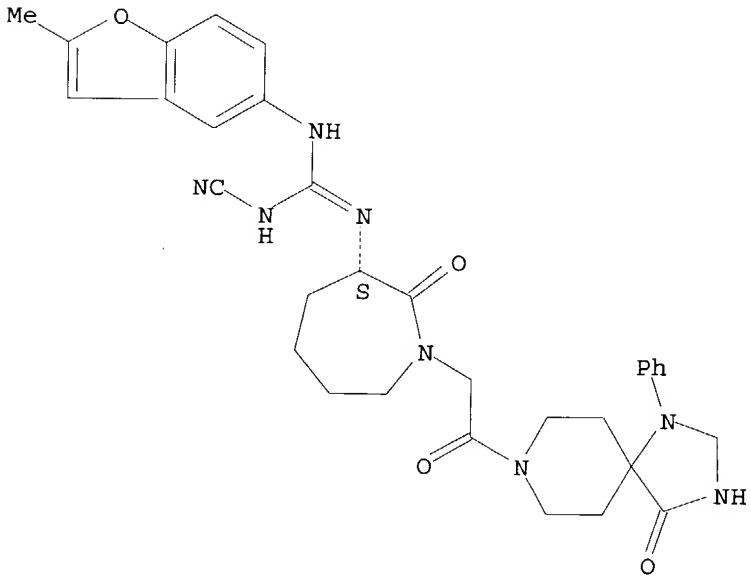
RN 288081-35-6 USPATFULL
CN Isoquinoline, 2-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

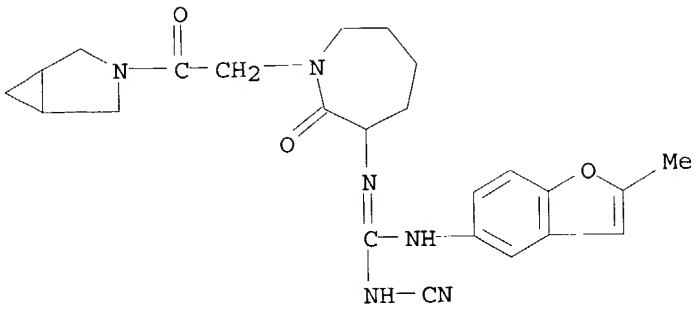


RN 288081-83-4 USPATFULL
CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[[(3S)-3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 288082-97-3 USPATFULL
CN 3-Azabicyclo[3.1.0]hexane, 3-[[3-[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)



L95 ANSWER 24 OF 30 USPATFULL on STN
ACCESSION NUMBER: 93:18665 USPATFULL
TITLE: Derivatives of 1,2,3,4-tetrahydronaphtylamine endowed with nootropic activity and pharmaceutical compositions containing same

INVENTOR(S): Giannessi, Fabio, Rome, Italy
Ghirardi, Orlando, Rome, Italy
Misiti, Domenico, Rome, Italy
Tinti, Maria O., Rome, Italy
Cozzolino, Roberto, Rome, Italy
PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite S.p.A., Rome, Italy (non-U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 5192759		19930309	
APPLICATION INFO.:	US 1991-809874		19911218	(7)

	NUMBER	DATE
PRIORITY INFORMATION:	IT 1990-48605	19901221

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Bond, Robert T.
LEGAL REPRESENTATIVE: Allegretti & Witcoff, Ltd.
NUMBER OF CLAIMS: 4
EXEMPLARY CLAIM: 1,3
LINE COUNT: 537

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB 1,2,3,4-tetrahydronaphthlamines of formula (1) ##STR1## wherein R is H or OCH.sub.3 ; ##STR2## is either at 1 or 2 position R.sub.1 is H;

R.sub.2 is selected from:

L-prolyl, optionally N-substituted with acetyl or carbobenzoxy,

L-pyroglutamyl,

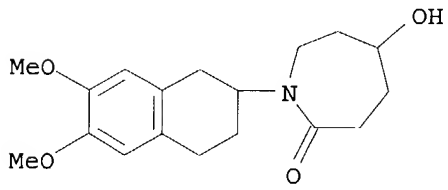
(pyrrolidin-2-one-1-yl)acetyl,

3-carboxy-2-hydroxypropyl:

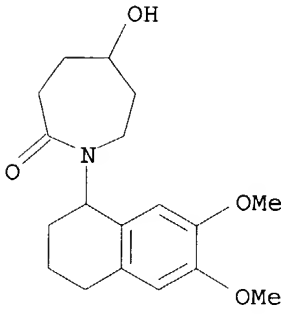
or R.sub.1 and R.sub.2 taken together with the nitrogen atom form the ring ##STR3## wherein n=1,2,3 and R.sub.3 -H, OH are nootropic substances potent enhancers of learning processes and memory.

Orally or parenterally administrable pharmaceutical compositions in unit dosage form comprise between about 100 and about 500 mg of a compound of formula (1).

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **143254-67-5P 143254-69-7P**
(preparation of)
RN 143254-67-5 USPATFULL
CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 143254-69-7 USPATFULL
CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)



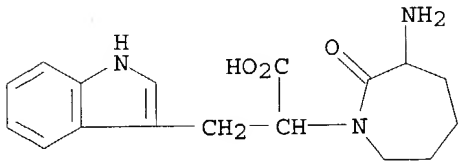
L95 ANSWER 25 OF 30 USPATFULL on STN
ACCESSION NUMBER: 87:50585 USPATFULL
TITLE: Substituted caprolactam derivatives as antihypertensives
INVENTOR(S): Harris, Elbert E., Westfield, NJ, United States
Patchett, Arthur A., Westfield, NJ, United States
Thorsett, Eugene D., Fanwood, NJ, United States
PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4680392		19870714
APPLICATION INFO.:	US 1986-864234		19860519 (6)

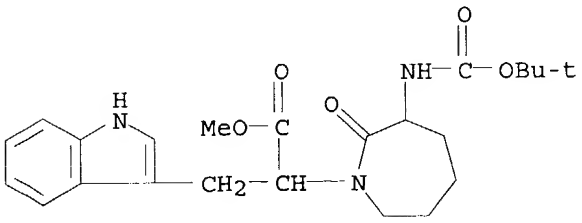
RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1982-394749, filed on 2 Jul 1982, now patented, Pat. No. US 4629787 which is a continuation-in-part of Ser. No. US 1981-282580, filed on 13 Jul 1981, now abandoned which is a continuation-in-part of Ser. No. US 1980-179305, filed

on 18 Aug 1980, now abandoned
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Bond, Robert T.
LEGAL REPRESENTATIVE: Mitri, Salvatore C., Sudol, Michael C., Monaco, Mario A.
NUMBER OF CLAIMS: 28
EXEMPLARY CLAIM: 1
LINE COUNT: 1662
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention in its broad aspects relates to caprolactam derivatives which are useful as angiotensin converting enxyme inhibitors and as antihypertensives.

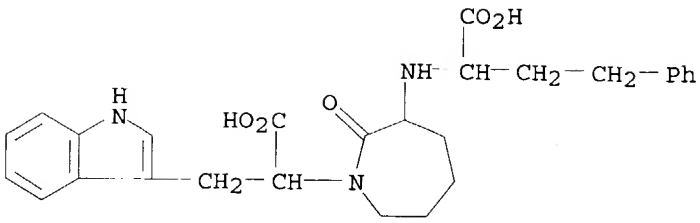
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **81867-57-4P**
(preparation and alkylation of)
RN 81867-57-4 USPATFULL
CN 1H-Indole-3-propanoic acid, α-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)- (9CI) (CA INDEX NAME)



IT **81867-56-3P**
(preparation and saponification of)
RN 81867-56-3 USPATFULL
CN 1H-Indole-3-propanoic acid, α-[3-[[(1,1-dimethylethoxy)carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]-, methyl ester (9CI) (CA INDEX NAME)



IT **81867-58-5P**
(preparation of)
RN 81867-58-5 USPATFULL
CN 1H-Indole-3-propanoic acid, α-[3-[(1-carboxy-3-phenylpropyl)amino]hexahydro-2-oxo-1H-azepin-1-yl]- (9CI) (CA INDEX NAME)



L95 ANSWER 26 OF 30 USPATFULL on STN

ACCESSION NUMBER:	86:71620 USPATFULL
TITLE:	Substituted caprolactam derivatives as antihypertensives
INVENTOR(S):	Harris, Elbert E., Westfield, NJ, United States Patchett, Arthur A., Westfield, NJ, United States Thorsett, Eugene D., Fanwood, NJ, United States
PATENT ASSIGNEE(S):	Merck & Co., Inc., Rahway, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4629787		19861216
APPLICATION INFO.:	US 1982-394749		19820702 (6)

RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1981-282580, filed on 13 Jul 1981, now abandoned which is a continuation-in-part of Ser. No. US 1980-179305, filed on 18 Aug 1980, now abandoned

DOCUMENT TYPE:	Utility
FILE SEGMENT:	Granted
PRIMARY EXAMINER:	Bond, Robert T.
LEGAL REPRESENTATIVE:	Mitri, Salvatore C., Sudol, Michael C.
NUMBER OF CLAIMS:	3
EXEMPLARY CLAIM:	1
LINE COUNT:	1484

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

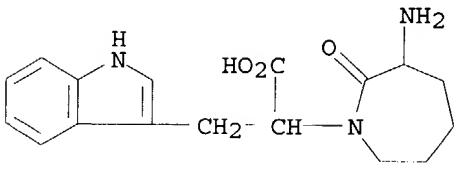
AB The invention in its broad aspects relates to caprolactam derivatives which are useful as angiotensin converting enxyme inhibitors and as antihypertensives.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **81867-57-4P**
(preparation and alkylation of)

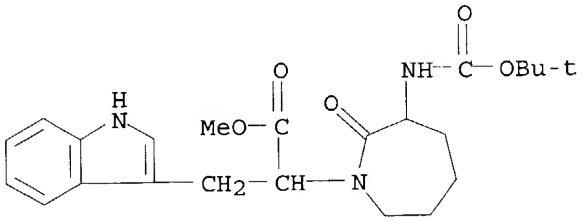
RN 81867-57-4 USPATFULL

CN 1H-Indole-3-propanoic acid, α-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)- (9CI) (CA INDEX NAME)

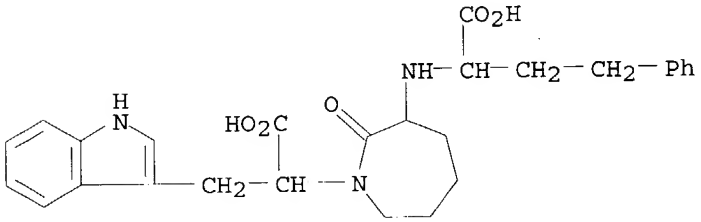


IT **81867-56-3P**
(preparation and saponification of)

RN 81867-56-3 USPATFULL
CN 1H-Indole-3-propanoic acid, α-[3-[[(1,1-dimethylethoxy)carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]-, methyl ester (9CI) (CA INDEX NAME)



IT **81867-58-5P**
(preparation of)
RN 81867-58-5 USPATFULL
CN 1H-Indole-3-propanoic acid, α-[3-[(1-carboxy-3-phenylpropyl)amino]hexahydro-2-oxo-1H-azepin-1-yl]- (9CI) (CA INDEX NAME)



L95 ANSWER 27 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:91887 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08905043156K
TITLE: Nitrosourea derivatives
AUTHOR(S): Matsumoto, Jun; Murakami, Masuo; Sato, Noriaki; Hashimoto, Shinichi; Kawamura, Tsutomu; Ichikawa, Kaichiro
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7834790 31 Mar 1978
SOURCE: (1978) Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1978:443156
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210

AB Nitrosourea derivs. I [R = 2-phenyl-2H-1,2,3-triazol-4-yl (II), 1-phenylpyrazol-5-yl, 4-methylphthalazan-3-yl, 1-adamantyl, 4-chloro-2-phenylpyrimidin-5-yl, Pr2NCO, 2,6-dioxopiperidin-4-ylmethyl, MeO2C] were prepared by silylation of III followed by reaction of RCOX (X = halo). I had antileukemic and anticarcinogenic activities (no data). Thus, 1.68 mL Et3N in dioxane was added to a mixture of 2.62 g III and 1.29 g Me3SiCl in dioxane, the whole stirred 20 h at room temperature, filtered, and

the filtrate concentrated to give 10 mL solution; 2-phenyl-1,2,3-triazol-4-carbonyl chloride (1.5 g) in CH2Cl2 was added to 6 mL of the solution and the mixture stirred 3 days at room temperature to give 165 mg II.

L95 ANSWER 28 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:65668 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08801006756Q
TITLE: Nitroso urea derivatives
AUTHOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Atsushi; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7783747 12 Jul 1977
SOURCE: (1977) Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1978:6756
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210

AB Twenty-eight title derivs. I [R = halo, substituted alkyl, (un)substituted alkenyl, (un)substituted aryl, (un)substituted heterocyclics; n = 2-10] were prepared by reaction of II with RCOX (X = halo). I had antitumor activity (some data given in mice). Thus, 174 mg 4-ClC6H4COCl in CHCl3 was added to 440 mg 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-nitrosourea mercuric salt in CHCl3 at room temperature and the mixture stirred 3 h to give 204 mg 1-(β-chloroethyl)-3-(N-p-chlorobenzoyl-2-oxo-3-hexahydroazepinyl)-1-nitrosourea.

L95 ANSWER 29 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:100440 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08717135119N
TITLE: 1-(β-Chloroethyl)-3-substituted 1-nitrosoureas
AUTHOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7751363 25 Apr 1977
SOURCE: (1977) Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1977:535119
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210

AB Thirteen title compds. (I, R = acyl) remedies for tumors, were prepared by treating non-substituted I with a silylating agent followed by acylation. Thus, 2.62 g 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-nitrosourea and Me3SiCl in dioxane were treated with NEt3 and treated with 352 mg p-[bis(β-chloroethyl)amino]benzoyl chloride in dichloromethane to give 403 mg I [R = p-[bis(β-chloroethyl)amino]benzoyl]. Among 12 I similarly prepared were (R given): 4-oxo-4H-thiopyran-3-carbonyl, p-O2NC6H4CO, p-(dimethylamino)benzoyl, 3-methyl-2-oxo-2,3-dihydrobenzothiazole-6-carbonyl.

L95 ANSWER 30 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:96931 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08713102197H
TITLE: Nitrosourea derivatives
AUTHOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7746072 12 Apr 1977
SOURCE: (1977) Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1977:502197
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210

AB Fifteen nitrosourea derivs. I [R1 = (un)substituted Ph, furyl, pyrazinyl, H2C:CH, PhCH2, ClCH2, etc.] were prepared by reaction of II with R1COX (X = halo). I had anticancer activity (some data given in mice). Thus, 124 mg 4-ClC6H4COCl in CHCl3 was added to 440 mg II HgCl2 salt in CHCl3 and the mixture stirred 3 h at room temperature to give 204 mg I (R1 = 4-ClC6H4).

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